Access DB# 215113

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Thuong Nguyen Examiner #: 69337 Date: 2/8/07
Art Unit: 1711 Phone Number 302-1681 Serial Number: 10/509,380
Mail Box and Bldg/Room Location: 6D71 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names): _____

Earliest Priority Filing Date: _____

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**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Either formula (I) or (II), related to the claimed method 1-
Thanks.

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NA Sequence (#) _____
AA Sequence (#) _____
Structure (#) _____
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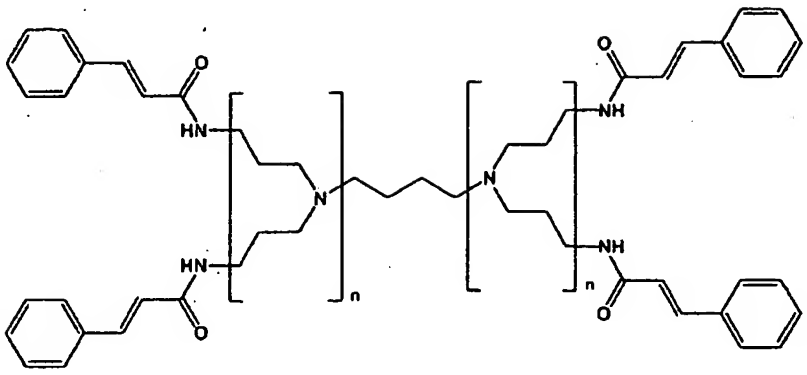
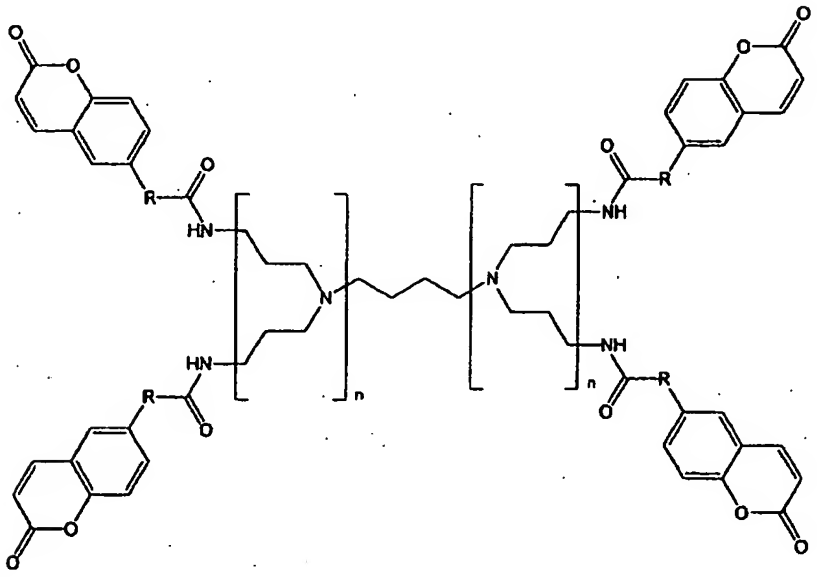
PTO-1590 (8-01)



(I)

wherein n represents an integer of 10 or less, and



(II)

wherein n represents an integer of 10 or less and R represents a linkage group.

AMENDMENTS TO THE CLAIMS

This listing of claims replaces all prior versions of claims in the application.

1. (Currently Amended): A method of producing a molecular device including:

a step of intra-molecule bonding by crosslinking [[the]] bonding residues ~~by using~~ in a molecular structure having a higher atomic density in the periphery than in the interior and having the bonding residues in the periphery.

2. (Currently Amended): The method of producing a molecular device according to claim 1, characterized in that the molecular structure is constituted by a skeleton portion having a skeleton structure, and a terminal portion which is arranged in [[the]] an outer shell of the skeleton portion, and the terminal portion has a higher atomic density than that of the skeleton portion and the terminal portion has bonding residues;

and that in the step of intra-molecule bonding by crosslinking the bonding residues, the bonding residues in the terminal portion of the molecular structure are crosslinked to form the molecular structure into a shell structure.

3. (Original): The method of producing a molecular device according to claim 1 or 2, wherein the bonding residue is an optically bonding residue.

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Bib Data Sheet

CONFIRMATION NO. 5055

SERIAL NUMBER	FILING OR 371(c) DATE	CLASS	GROUP ART UNIT	ATTORNEY DOCKET NO.
10/509,380	09/27/2004 RULE	528	1712	042757

APPLICANTS

Seiichi Furumi, Tokyo, JAPAN;
Akira Otomo, Tokyo, JAPAN;
Shinro Mashiko, Tokyo, JAPAN;

**** CONTINUING DATA ***************************

This application is a 371 of PCT/JP03/03669 03/26/2003

**** FOREIGN APPLICATIONS *********************

JAPAN 2002-91548 03/28/2002
JAPAN 2002-94211 03/29/2002

Foreign Priority claimed	STATE OR COUNTRY	SHEETS DRAWING	TOTAL CLAIMS	INDEPENDENT CLAIMS
☑ yes ☐ no	JAPAN	7	37	9
35 USC 119 (a-d) conditions met: ☑ yes ☐ no ☐ Met after Allowance				
Verified and Acknowledged: Examiner's Signature / Initials				

ADDRESS

38834

TITLE

Process for production of molecular devices

FILING FEE RECEIVED	FEES: Authority has been given in Paper	
2662	No. _____ to charge/credit DEPOSIT ACCOUNT No. _____ for following:	☐ All Fees ☐ 1.16 Fees (Filing) ☐ 1.17 Fees (Processing Ext. of time) ☐ 1.18 Fees (Issue) ☐ Other _____ ☐ Credit

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L1                STR
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L3                STR
L4                STR

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L6                STR L4
L7              3 S (L2 OR L3) AND L6

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L10           844 S MASHIKO ?/AU
L11            11 S L8 AND L9 AND L10
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L17               STR L2
L18             3 S (L17 OR L3) AND L6
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L20             1 S L19 AND L16
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L22             0 S L20
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     FILE 'ZCA'
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FILE 'REGISTRY'

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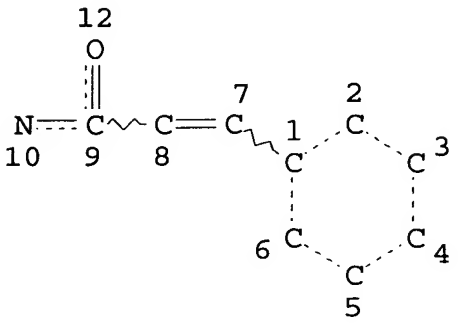

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DEFAULT ECLEVEL IS LIMITED

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STEREO ATTRIBUTES: NONE
L6 STR

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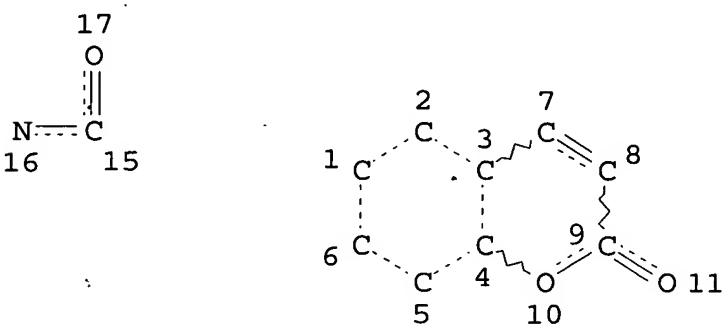

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L24 ANSWER 1 OF 1 ZCA COPYRIGHT 2007 ACS on STN
140:33496 Effective photocrosslinking reaction of dendrimers through triplet energy transfer. Furumi, Seiichi; Otomo, Akira; Yokoyama, Shiyoshi; Mashiko, Shinro (Communications Research Laboratory, Kasai Advanced Research Center, Nishi-ku, Kobe, 651-2492, Japan). Thin Solid Films, 438-439, 85-89 (English) 2003. CODEN: THSFAP. ISSN: 0040-6090. Publisher: Elsevier Science B.V..

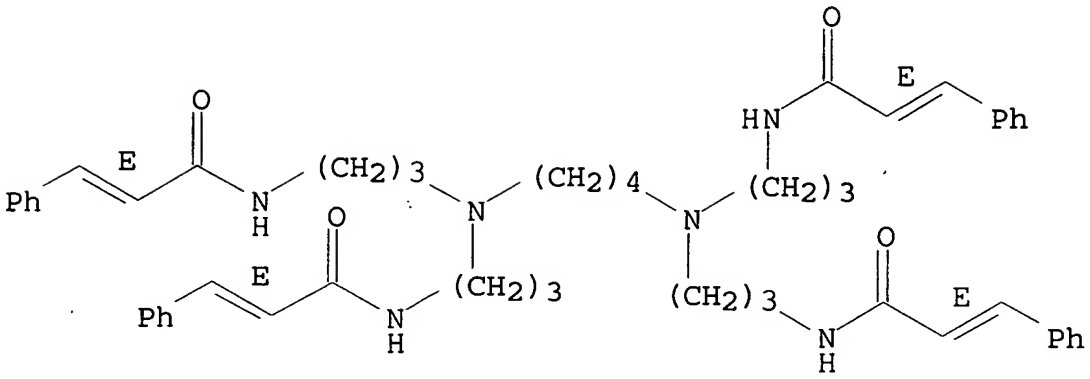
AB In this article, we describe the synthesis and photoreactions of photocrosslinkable dendrimers bearing trans-cinnamoyl residues at the peripheral positions. Photoirradn. of the dendrimers with 313 nm gave rise to monotonous decrease in the absorbance of trans-cinnamates at 270 nm as a result of their photochem. reactions involving trans-to-cis photoisomerization and [2+2] photodimerization. The first-generation dendrimer displayed the preferential formation of cis-cinnamates at the photostationary state, whereas the photodimerization took place favorably for the third- and fifth-generation dendrimers. The photodimerized rate was strongly dependent on the dendritic generation rather than the concn. of solns., probably due to the extent of steric crowding among the cinnamates settled on the dendritic surfaces. The third- and fifth-generation dendrimers enabled the capturing of a phosphorescent sensitizer into the internal dendritic cavities to generate the effective photocrosslinking of the cinnamates in an intramacromol. manner through triplet energy transfer from the excited sensitizer. The photocrosslinking reaction of dendrimers through the triplet energy transfer might provide potential applicabilities to design and fabricate novel optical and elec. mol. devices from the bottom-up approach.

IT **634179-50-3P**
(effective photocrosslinking reaction of dendrimers through triplet energy transfer)

RN 634179-50-3 ZCA

CN 2-Propenamide, N,N',N'',N'''-[1,4-butanediylbis(nitrilodi-3,1-propanediyl)]tetrakis[3-phenyl-, (2E,2'E,2''E,2'''E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT **634179-50-3P**
(effective photocrosslinking reaction of dendrimers through triplet energy transfer)

=> D L25 1-22 CBIB ABS HITSTR HITRN

L25 ANSWER 1 OF 22 ZCA COPYRIGHT 2007 ACS on STN
145:451267 Biosensors and methods for detecting agents based upon time resolved luminescent resonance energy transfer. Zahner, Joseph Edward (USA). U.S. Pat. Appl. Publ. US 2006240571 A1 20061026, 8pp. (English). CODEN: USXXCO. APPLICATION: US 2006-408529 20060420. PRIORITY: US 2005-673059P 20050420.

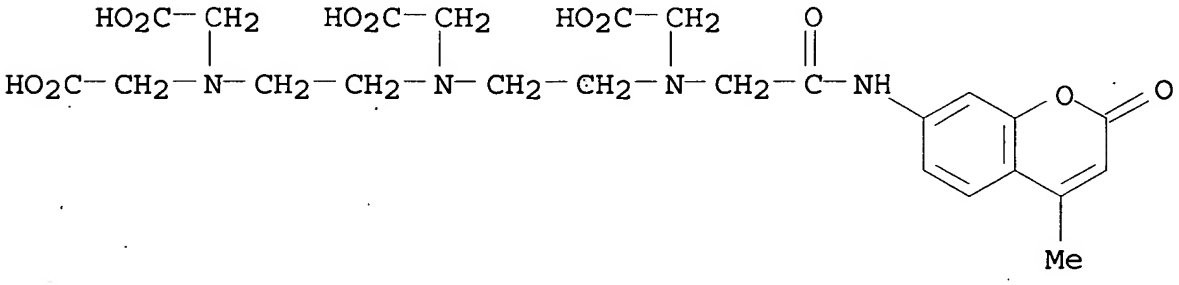
AB Disclosed are biosensors useful in the detection of potentially harmful or undesirable agents, particularly chems. and microorganisms in food and water. The biosensors operate under the principle of time-resolved luminescence resonance energy transfer. In a preferred embodiment, the biosensor comprises antibodies that recognized different but proximal epitopes on a particular agent. One antibody contains a luminescence donor that emits energy over time, such as a lanthanide series-based luminophor. Another antibody contains a luminescence acceptor that is excited by the emission spectrum of the donor and emits at a particular wavelength, such as for example the fluorophor Cy3. In the presence of the agent, the donor and acceptor are brought into close proximity, such that the energy transfer can occur. The donor is excited by a transient burst of light and the emitted wavelength is received by a photodiode, quantified and correlated to amt. of agent in a sample. For sensing Escherichia coli, monoclonal antibodies 15402 and 15403 were pooled and then conjugated with a terbium chelate and monoclonal antibodies 15404 and 15405 were pooled and conjugated with Cy3 monofunctional NHS ester and the labeled antibodies were contacted with sample solns. Within from five (5) to 15 min of mixing, each sample was subjected to 30 Hz of 5 ns pulses from a

nitrogen laser (337 nm). Between light pulses (hence--time resolved), light of 541 nm (terbium emission) and 570 nm (Cy3 emission) were measured. The ratio of 570/541 was detd. for each sample. A pos. correlation was found between no. of E. coli bacteria (X-axis) and adjusted 570/541 ratio (Y-axis). By adjusted, the baseline was set at 1.0, which is for the mixt. of the conjugates without any E. coli present.

IT **191661-03-7D**, reaction with terbium
(conjugation with monoclonal antibodies to Escherichia coli; biosensors and methods for detecting agents based upon time-resolved luminescent resonance energy transfer)

RN 191661-03-7 ZCA

CN Glycine, N-[2-[bis(carboxymethyl)amino]ethyl]-N-[2-[(carboxymethyl)[2-[(4-methyl-2-oxo-2H-1-benzopyran-7-yl)amino]-2-oxoethyl]amino]ethyl]- (9CI) (CA INDEX NAME)



IT **191661-03-7D**, reaction with terbium
(conjugation with monoclonal antibodies to Escherichia coli; biosensors and methods for detecting agents based upon time-resolved luminescent resonance energy transfer)

L25 ANSWER 2 OF 22 ZCA COPYRIGHT 2007 ACS on STN

144:288565 Luminescent metal complexes for monitoring renal function. Rajagopalan, Raghavan; Dorshow, Richard B.; Moore, Dennis A. (Mallinckrodt Inc., USA). PCT Int. Appl. WO 2006026038 A1 20060309, 42 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IS, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2005-US27486 20050803. PRIORITY: US 2004-604573P 20040826.

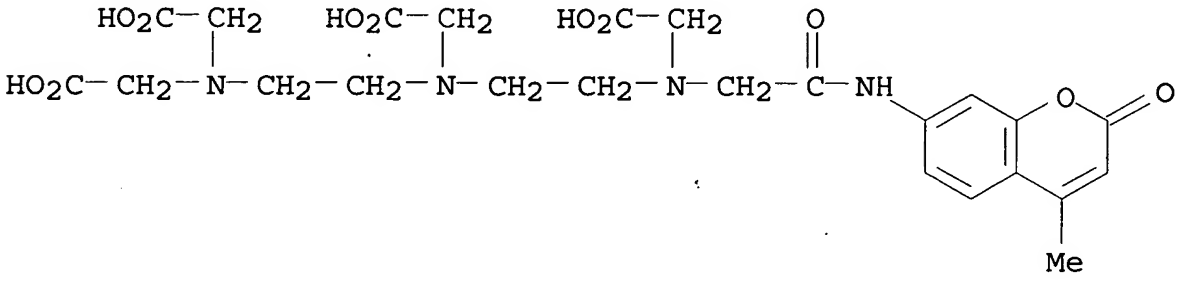
AB The present invention relates to fluorescent DTPA metal complexes, corresponding DTPA ligands, and methods of monitoring renal function using such metal complexes. Examples of 111In complexes and their

biodistribution and hepatobiliary clearance are provided.

IT **191661-03-7**
(complexes of 111In with DTPA derivs. as kidney imaging agents)

RN 191661-03-7 ZCA

CN Glycine, N-[2-[bis(carboxymethyl)amino]ethyl]-N-[2-[(carboxymethyl)[2-[(4-methyl-2-oxo-2H-1-benzopyran-7-yl)amino]-2-oxoethyl]amino]ethyl]- (9CI) (CA INDEX NAME)



IT **191661-03-7**
(complexes of 111In with DTPA derivs. as kidney imaging agents)

L25 ANSWER 3 OF 22 ZCA COPYRIGHT 2007 ACS on STN

144:88556 Preparation of tetramines for activation of binding of p53 to DNA. Sato, Masakazu; Wada, Hisaya; Amada, Hideaki (Taisho Pharmaceutical Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2006008533 A 20060112, 36 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2004-184095 20040622.

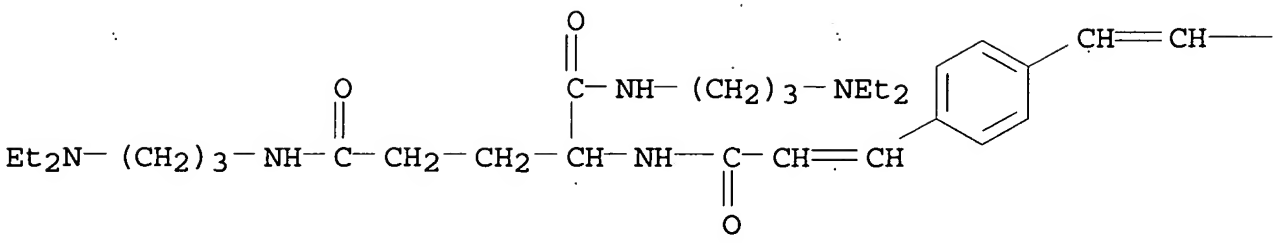
AB A[CONHCHZ(CH2)mZ]2 [Z = CONH(CH2)nNR1R2; R1, R2 = H, C1-6 alkyl; R1NR2 may form satd. heterocyclyl; n = 1-5; m = 1, 2; A = substituted (cyclo)alkylene, naphthalenediyl, substituted xanthenediyl, etc.] or their medically acceptable salts, useful for induction of apoptosis in tumor cells, are prepd. Thus, Z-Glu was amidated with Et2N(CH2)3NH2, deprotected, and refluxed with 2,4,5,6-tetrafluoroisophthaloyl dichloride to give tetramine, which at 100 μM showed 78.4% activation of binding of recombinant human p53 protein to DNA by Pab421 epitope peptide assay.

IT **872460-99-6P 872461-10-4P 872461-24-0P**
872461-27-3P
(prepn. of tetramines as antitumor agents)

RN 872460-99-6 ZCA

CN Pentanediamide, 2,2'-[1,4-phenylenebis[(1-oxo-2-propene-3,1-diyl)imino]]bis[N,N'-bis[3-(diethylamino)propyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



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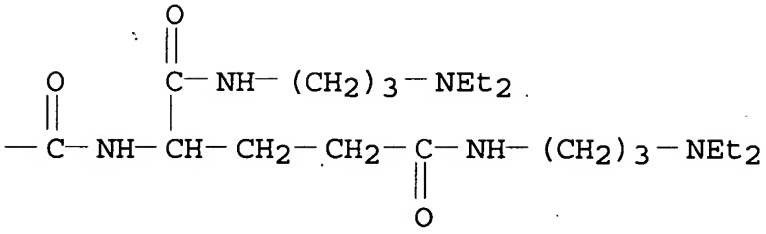
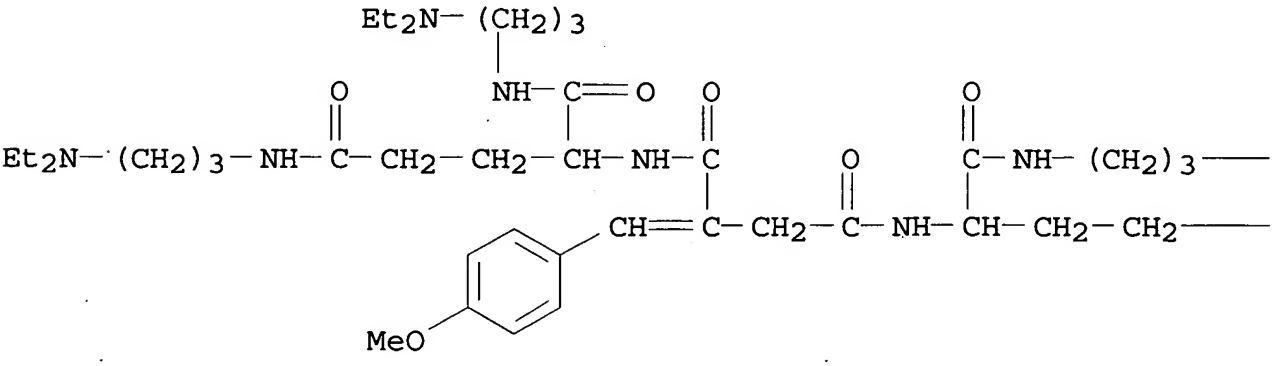


RN 872461-10-4 ZCA
CN Pentanediamide, 2,2'-[[2-[(4-methoxyphenyl)methylene]-1,4-dioxo-1,4-butanediyl]diimino]bis[N,N'-bis[3-(diethylamino)propyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



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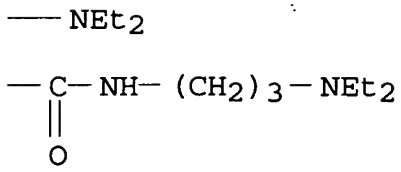
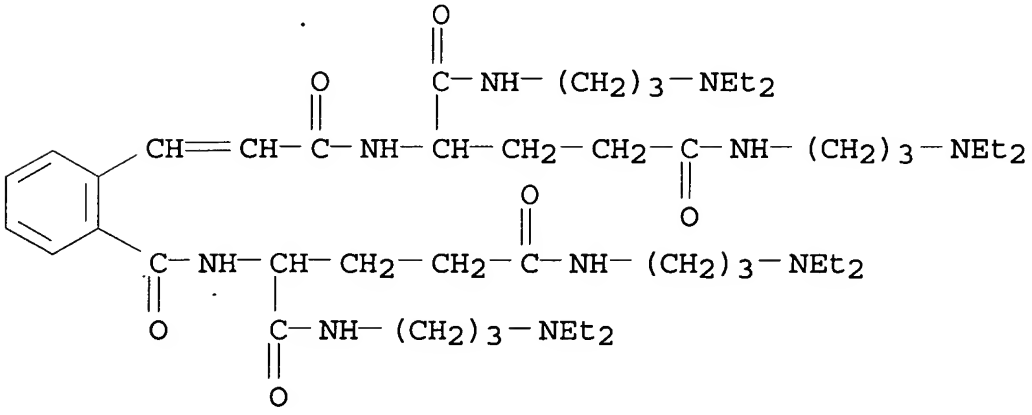
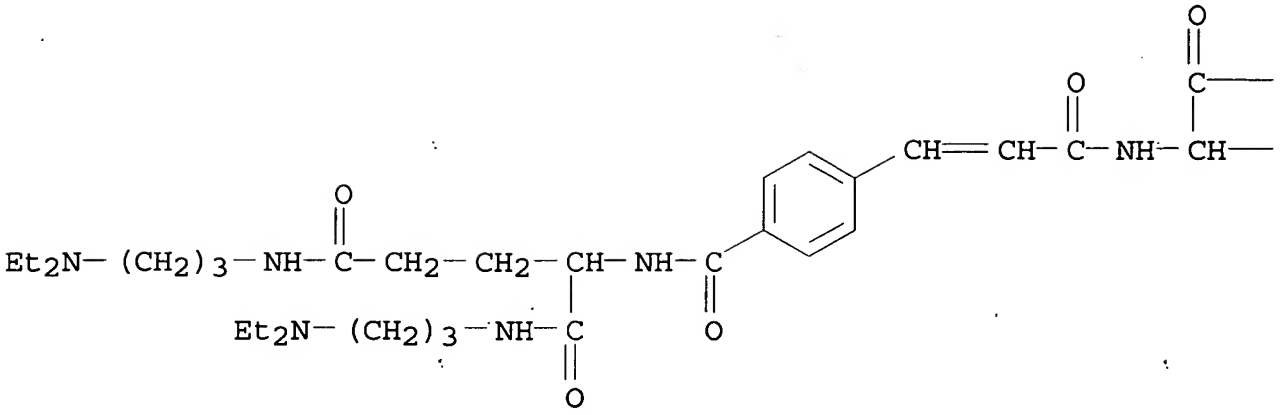


RN 872461-24-0 ZCA
CN Pentanediamide, N,N'-bis[3-(diethylamino)propyl]-2-[[3-[2-[[[4-[[3-(diethylamino)propyl]amino]-1-[[[3-(diethylamino)propyl]amino]carbonyl]-4-oxobutyl]amino]carbonyl]phenyl]-1-oxo-2-propenyl]amino]- (9CI) (CA INDEX NAME)



RN 872461-27-3 ZCA
CN Pentanediamide, N,N'-bis[3-(diethylamino)propyl]-2-[[3-[4-[[[4-[[3-(diethylamino)propyl]amino]-1-[[[3-(diethylamino)propyl]amino]carbonyl]-4-oxobutyl]amino]carbonyl]phenyl]-1-oxo-2-propenyl]amino]- (9CI) (CA INDEX NAME)

PAGE 1-A



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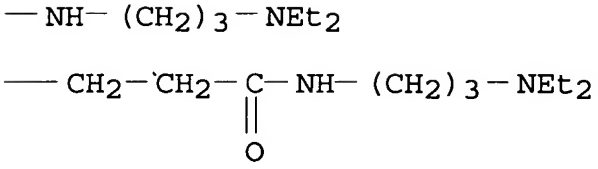

IT **872460-99-6P 872461-10-4P 872461-24-0P**
872461-27-3P
(prepn. of tetramines as antitumor agents)

L25 ANSWER 4 OF 22 ZCA COPYRIGHT 2007 ACS on STN
143:440266 Preparation of coumarin derivatives, Maillard reaction inhibitors containing them, and their uses for treatment of diabetic complications, skin aging, etc.. Hasegawa, Taisuke; Okubo, Tomohiro; Shibayama, Yoji; Furukawa, Kazuto (Nippon Zoki Pharmaceutical Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2005314240 A 20051110, 34 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2004-131408 20040427.
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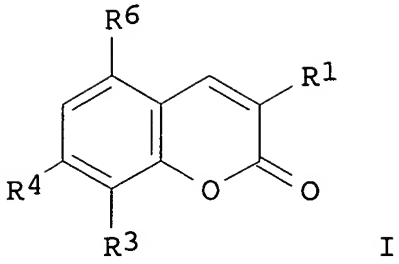


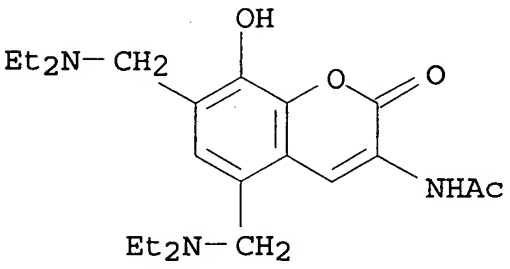
I

AB Coumarin derivs. I [R1 = NHX, COY; (X = H, Ac, CH2Ph; Y = alkyl, Ph, OH, alkoxy, amino optionally substituted with alkyl); R3 = OH, OAc; R4, R6 = H, aryl, N,N-dialkylaminoalkyl, piperidinoalkyl, morpholinoalkyl, imidazolylalkyl, (un)substituted piperazinoalkyl; if X = H or Ac and Y = alkoxy, then R4, R6 ≠ H] and their pharmacol. acceptable salts are prepd. Also claimed are prophylactic/therapeutic agents for diabetic complications, prophylactic/therapeutic agents for complications in hemodialysis, skin aging inhibitors, cosmetics, and discoloration/deterioration inhibitors contg. the Maillard reaction inhibitors. Thus, a mixt. of 2,3-(HO)2C6H3CHO, malonic acid, aniline, and pyridine was heated to dissolve and let stand at room temp. for 13% 8-hydroxy-2-oxo-2H-1-benzopyran-3-carboxylic acid. This showed 55.2% inhibition against formation of a protein dimer from lysozyme and glucose in sodium phosphate buffer (pH 7.4) upon heating at 45° for 3 days.

IT **868762-46-3P 868762-50-9P 868762-52-1P**
868762-54-3P
(prepn. of coumarin derivs. as Maillard reaction inhibitors and their use for treatment of diabetic complications, hemodialysis complications, skin aging, etc.)

RN 868762-46-3 ZCA

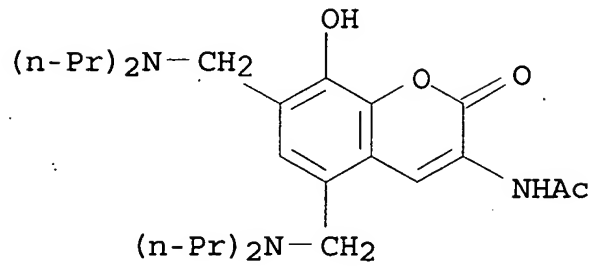
CN Acetamide, N-[5,7-bis[(diethylamino)methyl]-8-hydroxy-2-oxo-2H-1-benzopyran-3-yl]- (9CI) (CA INDEX NAME)



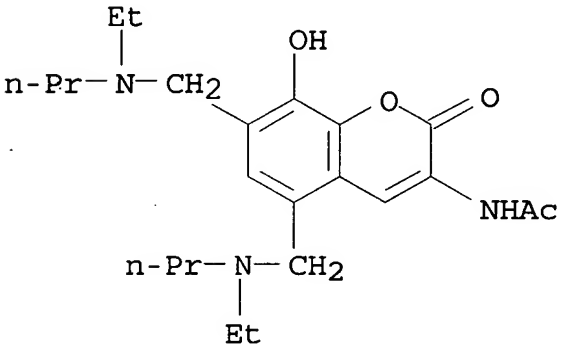
RN 868762-50-9 ZCA

CN Acetamide, N-[5,7-bis[(dipropylamino)methyl]-8-hydroxy-2-oxo-2H-1-

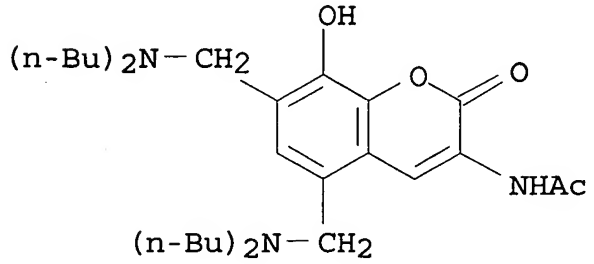
benzopyran-3-yl]- (9CI) (CA INDEX NAME)



RN 868762-52-1 ZCA
CN Acetamide, N-[5,7-bis[(ethylpropylamino)methyl]-8-hydroxy-2-oxo-2H-1-benzopyran-3-yl]- (9CI) (CA INDEX NAME)



RN 868762-54-3 ZCA
CN Acetamide, N-[5,7-bis[(dibutylamino)methyl]-8-hydroxy-2-oxo-2H-1-benzopyran-3-yl]- (9CI) (CA INDEX NAME)



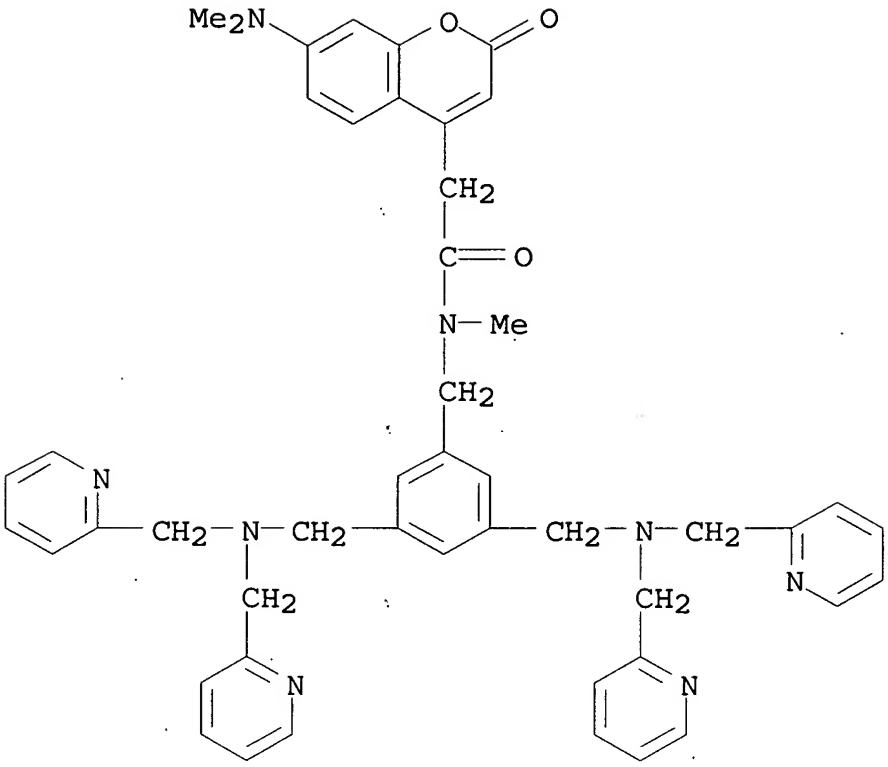
IT **868762-46-3P 868762-50-9P 868762-52-1P 868762-54-3P**
(prepn. of coumarin derivs. as Maillard reaction inhibitors and their use for treatment of diabetic complications, hemodialysis complications, skin aging, etc.)

L25 ANSWER 5 OF 22 ZCA COPYRIGHT 2007 ACS on STN
143:301538 Cooperation between Artificial Receptors and Supramolecular Hydrogels for Sensing and Discriminating Phosphate Derivatives. Yamaguchi, Satoshi; Yoshimura, Ibuki; Kohira, Takahiro; Tamaru, Shunichi; Hamachi, Itaru (PRESTO (Synthesis and Control Japan Science and Technology) Department of Synthetic Chemistry and Biological Chemistry, Kyoto University, Kyoto, 615-8510, Japan). Journal of the American Chemical Society, 127(33), 11835-11841 (English) 2005. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 143:301538. Publisher: American Chemical Society.

AB This study has successfully demonstrated that the cooperative action of artificial receptors with semi-wet supramol. hydrogels may produce a unique and efficient mol. recognition device not only for the simple sensing of phosphate derivs., but also for discriminating among phosphate derivs. The authors directly obsd. by confocal laser scanning microscopy that fluorescent artificial receptors can dynamically change the location between the aq. cavity and the hydrophobic fibers upon guest-binding under semi-wet conditions provided by the supramol. hydrogel. On the basis of such a guest-dependent dynamic redistribution of the receptor mols., a sophisticated means for mol. recognition of phosphate derivs. can be rationally designed in the hydrogel matrix. That is, the elaborate utilization of the hydrophobic fibrous domains, as well as the water-rich hydrophilic cavities, enables the authors to establish three distinct signal transduction modes for phosphate sensing: the use of (i) a photoinduced electron transfer type of chemosensor, (ii) an environmentally sensitive probe, and (iii) an artificial receptor displaying a fluorescence resonance energy transfer type of fluorescent signal change. Thus, one can selectively sense and discriminate the various phosphate derivs., such as phosphate, phospho-tyrosine, Ph phosphate, and ATP, using a fluorescence wavelength shift and a seesaw type of ratiometric fluorescence change, as well as a simple fluorescence intensity change. It is also shown that an array of the miniaturized hydrogel is promising for the rapid and high-throughput sensing of these phosphate derivs.

IT **864685-61-0P**
(cooperation between artificial receptors and supramol. hydrogels for sensing and discriminating phosphate derivs. in relation to synthesis of receptors)

RN 864685-61-0 ZCA
CN 2H-1-Benzopyran-4-acetamide, N-[[3,5-bis[[bis(2-pyridinylmethyl)amino]methyl]phenyl]methyl]-7-(dimethylamino)-N-methyl-2-oxo- (9CI) (CA INDEX NAME)



IT **864685-61-0P**
(cooperation between artificial receptors and supramol. hydrogels for sensing and discriminating phosphate derivs. in relation to synthesis of receptors)

L25 ANSWER 6 OF 22 ZCA COPYRIGHT 2007 ACS on STN
143:3598 Esterase-activated two-fluorophore system for ratiometric sensing of biological zinc(II). Woodroofe, Carolyn C.; Won, Annie C.; Lippard, Stephen J. (Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA). Inorganic Chemistry, 44(9), 3112-3120 (English) 2005. CODEN: INOCAJ. ISSN: 0020-1669. Publisher: American Chemical Society.

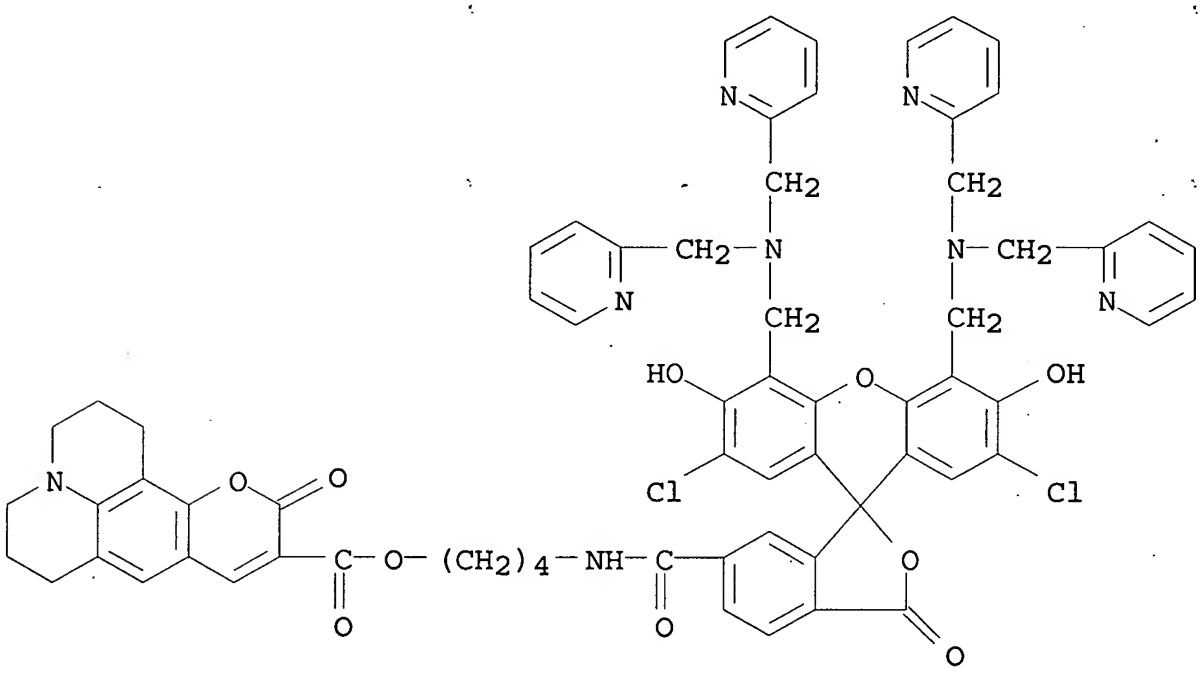
AB Intracellular ester hydrolysis by cytosolic esterases is a common strategy used to trap fluorescent sensors within the cell. We have prepd. analogs of Zinpyr-1 (ZP1), an intensity-based fluorescent sensor for Zn2+, that are linked via an amido-ester or diester moiety to a calibrating fluorophore, coumarin 343. These compds., designated Coumazin-1 and -2, are nonpolar and are quenched by intramol. interactions between the two fluorophores. Esterase-catalyzed hydrolysis generates a Zn2+-sensitive ZP1-like fluorophore and a Zn2+-insensitive coumarin as a calibrating fluorophore. Upon excitation of the fluorophores, coumarin 343 emission relays information concerning sensor concn. whereas ZP1

emission indicates the relative concn. of Zn2+-bound sensor. This approach enables intracellular monitoring of total sensor concn. and provides a ratiometric system for sensing biol. zinc ion.

IT **852299-72-0P**
(esterase-activated two-fluorophore system for ratiometric sensing of biol. zinc(II))

RN 852299-72-0 ZCA

CN 1H,5H,11H-[1]Benzopyrano[6,7,8-ij]quinolizine-10-carboxylic acid, 2,3,6,7-tetrahydro-11-oxo-, 4-[[[4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl]carbonyl]amino]butyl ester (9CI) (CA INDEX NAME)



IT **852299-72-0P**
(esterase-activated two-fluorophore system for ratiometric sensing of biol. zinc(II))

L25 ANSWER 7 OF 22 ZCA COPYRIGHT 2007 ACS on STN

142:332455 Multiplex binding and activity assays. Vogel, Kurt (Invitrogen Corporation, USA). PCT Int. Appl. WO 2005026730 A2 20050324, 90 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN,

YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2004-US29099 20040908. PRIORITY: US 2003-502377P 20030912.

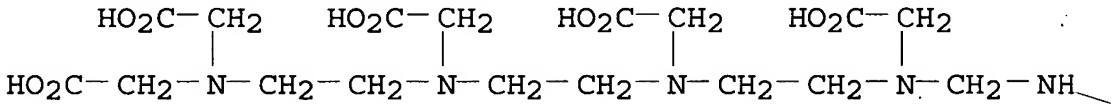
AB Compns., including antibodies, polypeptides, and org. mols., kits, apparatuses, and methods for probing mol. interactions using fluorescence polarization (FP) and/or time-resolved resonance energy transfer (TR-RET) are provided.

IT **848125-19-9D**, europium complex
(multiplex binding and activity assays)

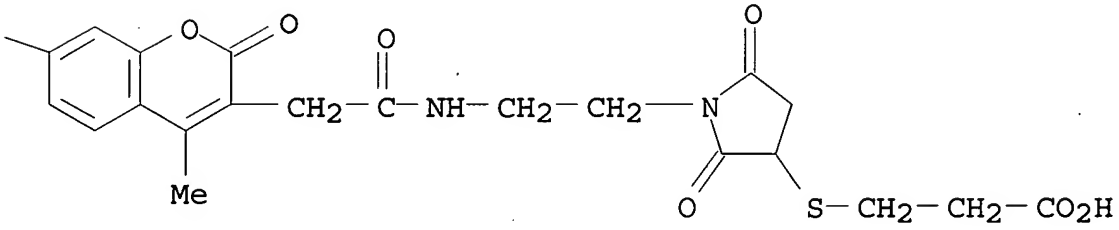
RN 848125-19-9 ZCA

CN 3,6,9,12-Tetraazatetradecanedioic acid, 3-[[[3-[2-[[2-[3-[(2-carboxyethyl)thio]-2,5-dioxo-1-pyrrolidinyl]ethyl]amino]-2-oxoethyl]-4-methyl-2-oxo-2H-1-benzopyran-7-yl]amino]methyl]-6,9,12-tris(carboxymethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



IT **848125-19-9D**, europium complex
(multiplex binding and activity assays)

L25 ANSWER 8 OF 22 ZCA COPYRIGHT 2007 ACS on STN

140:391166 Product class 4: benzopyranones and benzopyranthiones. Williams, A. C.; Camp, N. (Germany). Science of Synthesis, 14, 347-638 (English) 2003. CODEN: SSCYJ9. Publisher: Georg Thieme Verlag.

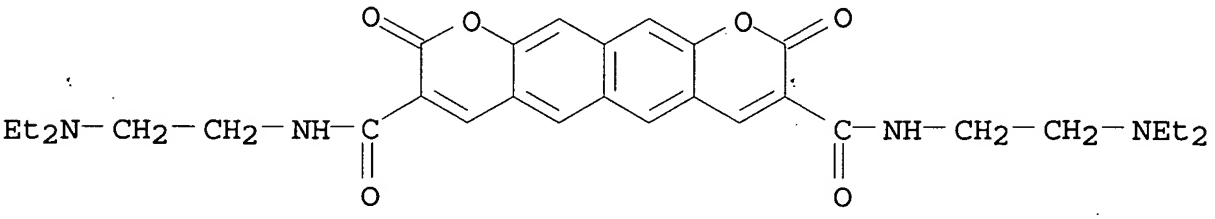
AB A review. Methods for prepg. 2H-1-benzopyran-2-ones, 4H-1-benzopyran-4-ones, 1H-2-benzopyran-1-ones, 6H-dibenzo[b,d]pyran-6-ones, 9H-xanthenones and their corresponding thione analogs as

well as 3H-2-benzopyran-3-ones are surveyed. Synthetic methods include ring closure, ring transformation, aromatization and substituent modification reactions.

IT **226561-46-2P**
(prepn. of benzopyranones and benzopyranthiones via ring closure, ring transformations, aromatization and substituent modifications)

RN 226561-46-2 ZCA

CN 2H,9H-Naphtho[2,3-b:7,6-b']dipyran-3,8-dicarboxamide, N,N'-bis[2-(diethylamino)ethyl]-2,9-dioxo- (9CI) (CA INDEX NAME)

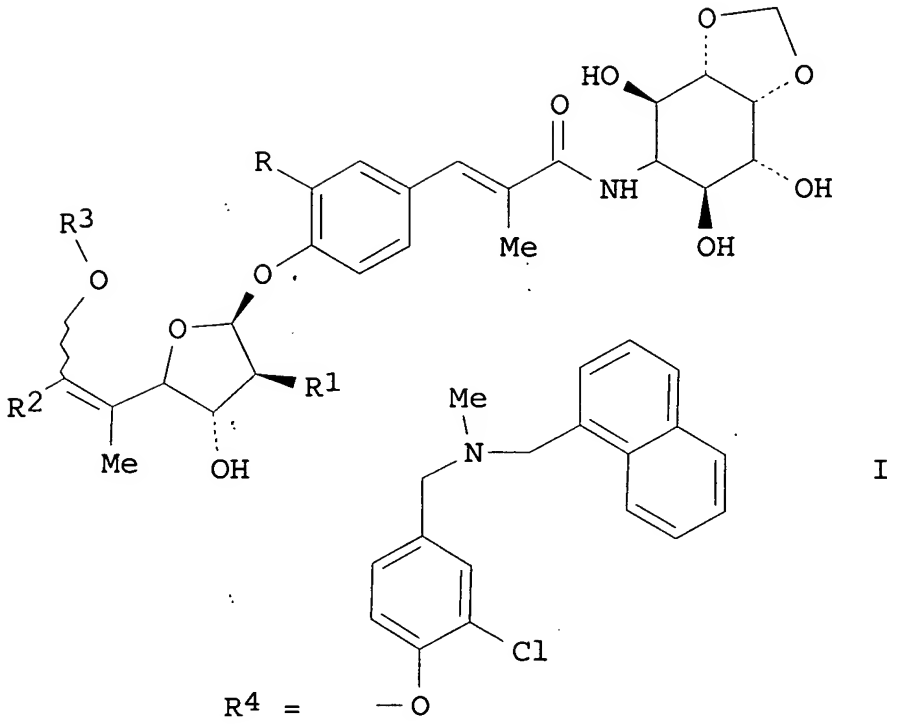


IT **226561-46-2P**
(prepn. of benzopyranones and benzopyranthiones via ring closure, ring transformations, aromatization and substituent modifications)

L25 ANSWER 9 OF 22 ZCA COPYRIGHT 2007 ACS on STN

136:6292 Preparation of hygromycin A derivatives for the treatment of bacterial and protozoal infections. Hayward, Matthew Merrill; Linde, Robert Gerald, II; Kaneko, Takushi; Visser, Michael Scott (Pfizer Products Inc., USA). PCT Int. Appl. WO 2001092280 A1 20011206, 112 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-IB946 20010525. PRIORITY: US 2000-209023P 20000602.

GI



I

AB Compds. I wherein R and R1 are independently H, OH; R2 is H, alkyl; R3 independently (un)substituted aryl, heteroarom., aminoalkyl, were prepd. for the treatment of bacterial and protozoal infections (no data). Compds. I are antibacterial and antiprotozoal agents that may be used to treat various bacterial and protozoal infections and disorders related to such infections (no data). Thus, I (R = R1 = OH, R2 = Me, R3 = R4) was prepd. from hygromycin and the use of Streptomyces hygroscopicus via Wittig reaction.

IT **377069-96-0P 377069-97-1P 377070-12-7P**
377070-13-8P 377070-14-9P 377070-15-0P
377070-16-1P 377070-17-2P 377070-18-3P
377070-19-4P 377070-20-7P 377070-21-8P
377072-42-9P
(prepn. of hygromycin A derivs. via Wittig reaction for the treatment of bacterial and protozoal infections)

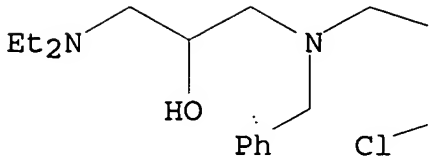
RN 377069-96-0 ZCA

CN D-neo-Inositol, 5-deoxy-5-[[(2E)-3-[4-[[(5E)-5,6-dideoxy-7-O-[2,3-dichloro-4-[[[3-(diethylamino)-2-hydroxypropyl](phenylmethyl)amino]methyl]phenyl]-5-methyl-β-D-arabino-hept-5-enofuranosyl]oxy]-3-hydroxyphenyl]-2-methyl-1-oxo-2-propenyl]amino]-1,2-O-methylene- (9CI) (CA INDEX NAME)

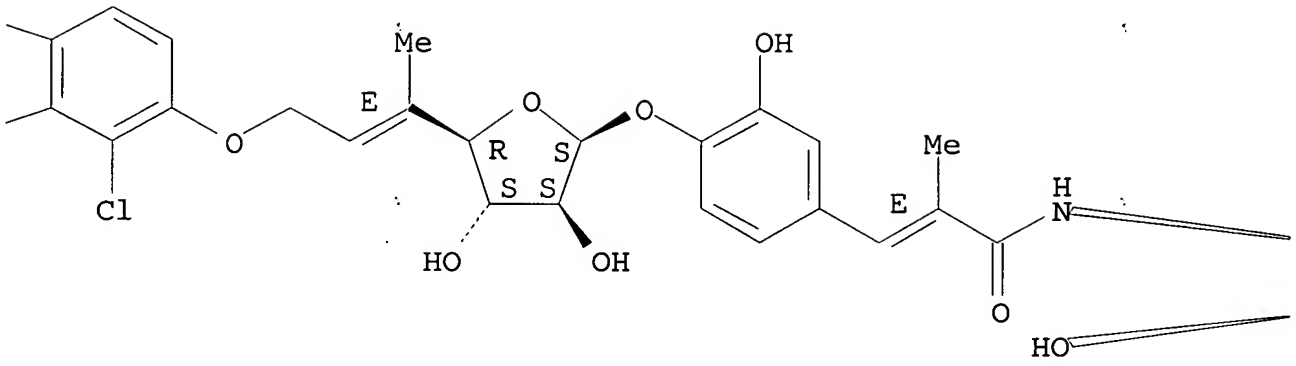
Absolute stereochemistry.

Double bond geometry as shown.

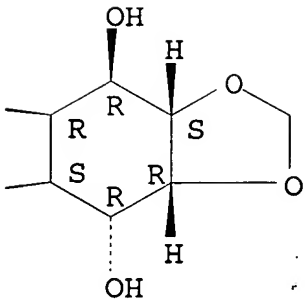
PAGE 1-A



PAGE 1-B



PAGE 1-C



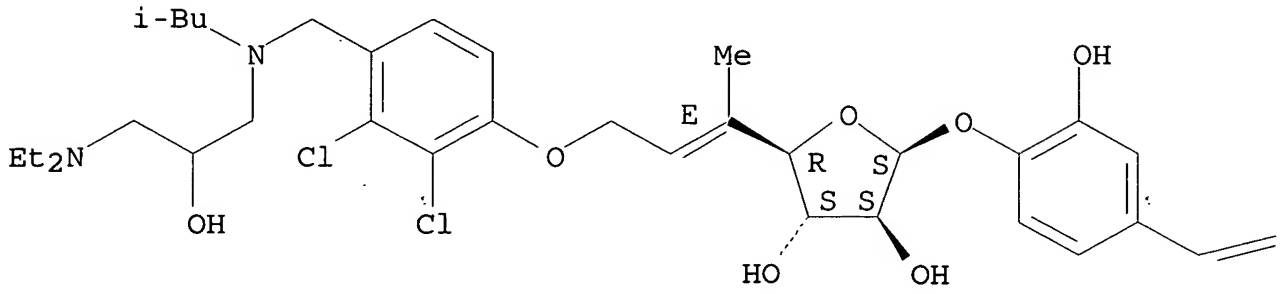
RN 377069-97-1 ZCA

CN D-neo-Inositol, 5-deoxy-5-[[(2E)-3-[4-[[(5E)-5,6-dideoxy-7-O-[2,3-dichloro-4-[[[3-(diethylamino)-2-hydroxypropyl](2-methylpropyl)amino]methyl]phenyl]-5-methyl-β-D-arabino-hept-5-

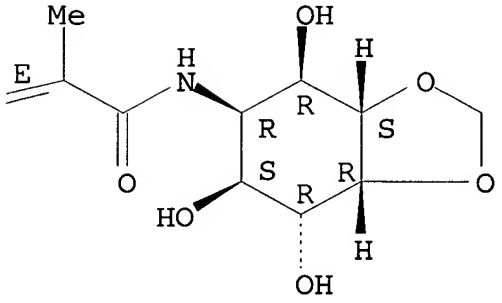
enofuranosyl]oxy]-3-hydroxyphenyl]-2-methyl-1-oxo-2-propenyl]amino]-1,2-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



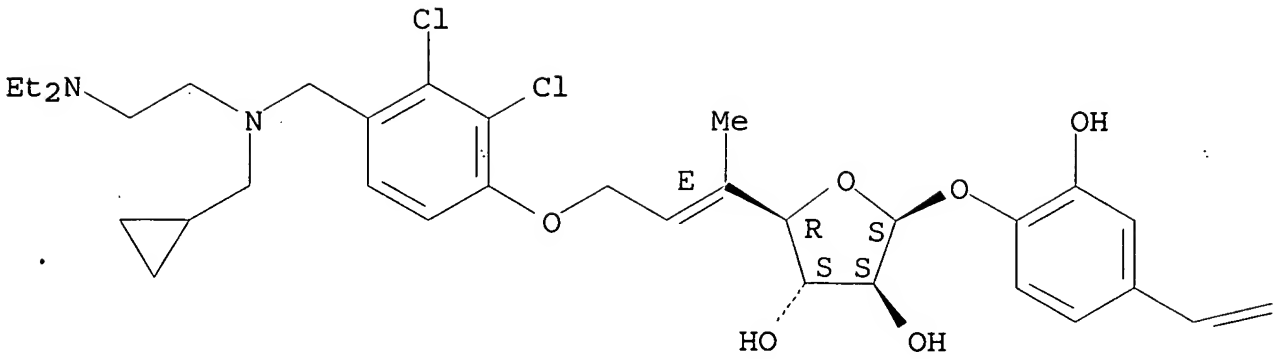
PAGE 1-B



RN 377070-12-7 ZCA
CN D-neo-Inositol, 5-deoxy-5-[[(2E)-3-[4-[[(5E)-5,6-dideoxy-7-O-[2,3-dichloro-4-[[(cyclopropylmethyl)[2-(diethylamino)ethyl]amino]methyl]phenyl]-5-methyl-β-D-arabino-hept-5-enofuranosyl]oxy]-3-hydroxyphenyl]-2-methyl-1-oxo-2-propenyl]amino]-1,2-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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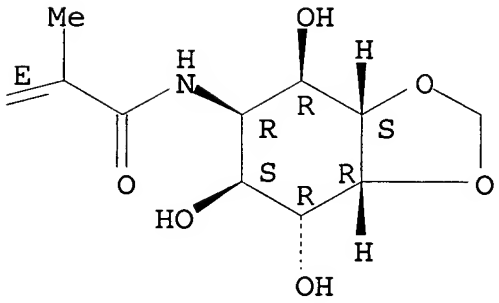
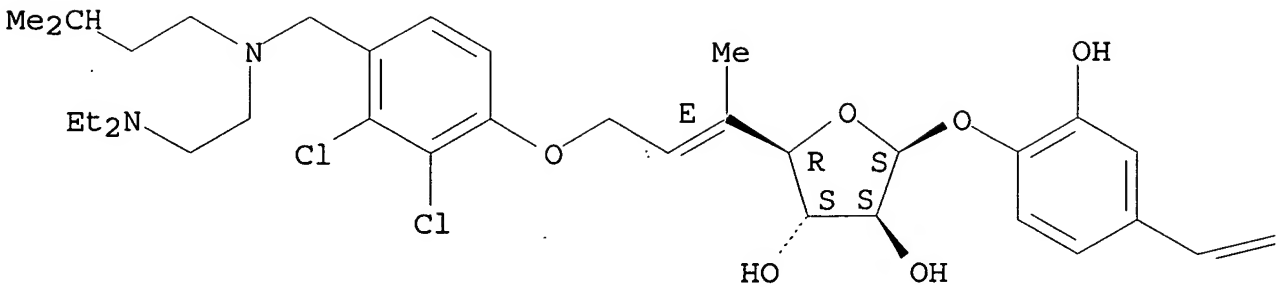


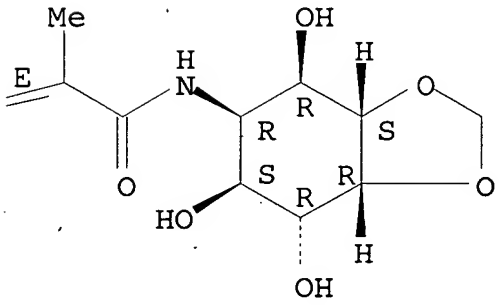
RN 377070-13-8 ZCA
CN D-neo-Inositol, 5-deoxy-5-[[(2E)-3-[4-[[(5E)-5,6-dideoxy-7-O-[2,3-dichloro-4-[[[2-(diethylamino)ethyl](3-methylbutyl)amino]methyl]phenyl]-5-methyl-β-D-arabino-hept-5-enofuranosyl]oxy]-3-hydroxyphenyl]-2-methyl-1-oxo-2-propenyl]amino]-1,2-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

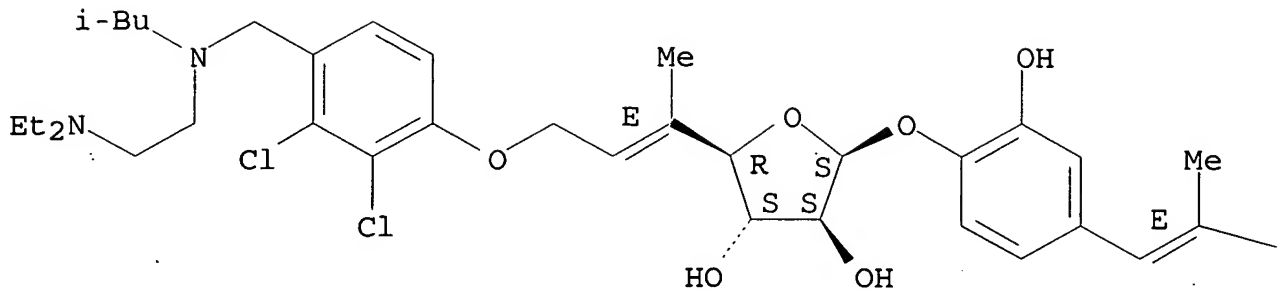


RN 377070-14-9 ZCA

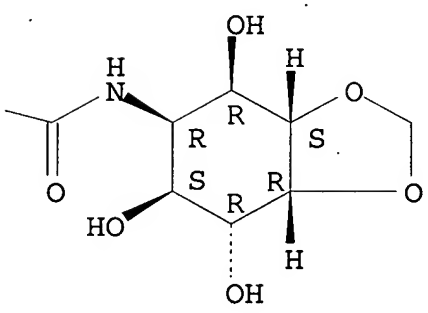
CN D-neo-Inositol, 5-deoxy-5-[[(2E)-3-[4-[[(5E)-5,6-dideoxy-7-O-[2,3-dichloro-4-[[[2-(diethylamino)ethyl](2-methylpropyl)amino]methyl]phenyl]-5-methyl-β-D-arabino-hept-5-enofuranosyl]oxy]-3-hydroxyphenyl]-2-methyl-1-oxo-2-propenyl]amino]-1,2-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



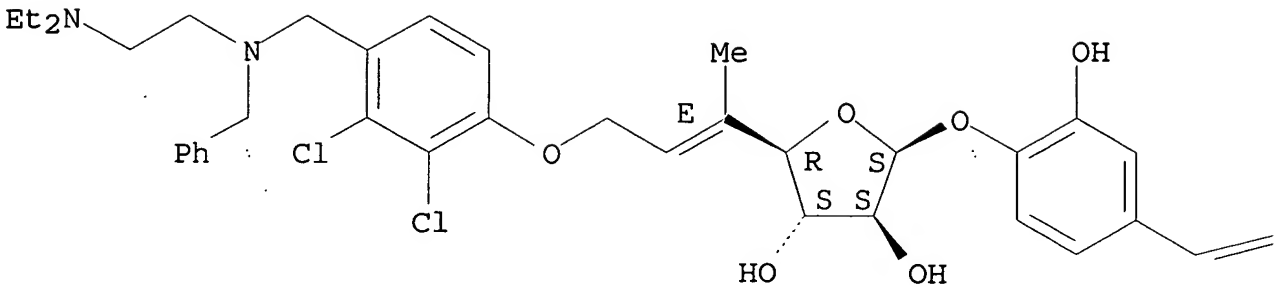
PAGE 1-B



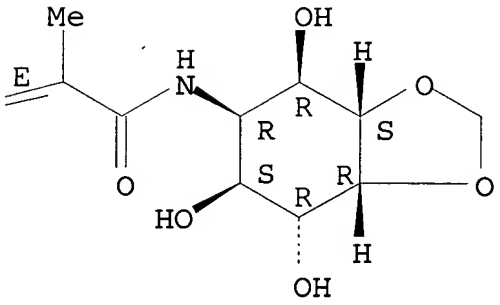
RN 377070-15-0 ZCA
CN D-neo-Inositol, 5-deoxy-5-[[(2E)-3-[4-[[(5E)-5,6-dideoxy-7-O-[2,3-dichloro-4-[[[2-(diethylamino)ethyl](phenylmethyl)amino]methyl]phenyl]-5-methyl-β-D-arabino-hept-5-enofuranosyl]oxy]-3-hydroxyphenyl]-2-methyl-1-oxo-2-propenyl]amino]-1,2-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



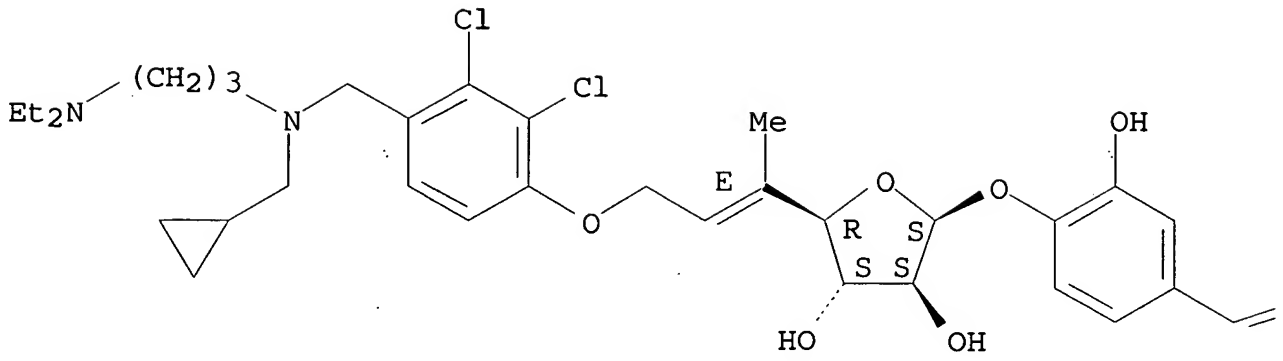
PAGE 1-B



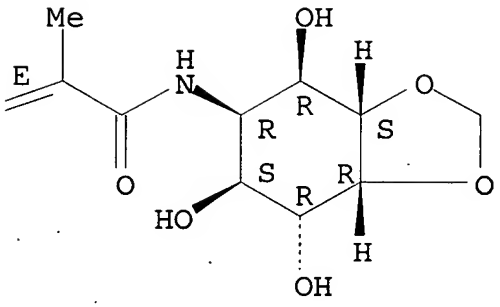
RN 377070-16-1 ZCA
CN D-neo-Inositol, 5-deoxy-5-[[(2E)-3-[4-[[(5E)-5,6-dideoxy-7-O-[2,3-dichloro-4-[[(cyclopropylmethyl)[3-(diethylamino)propyl]amino]methyl]phenyl]-5-methyl-β-D-arabino-hept-5-enofuranosyl]oxy]-3-hydroxyphenyl]-2-methyl-1-oxo-2-propenyl]amino]-1,2-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



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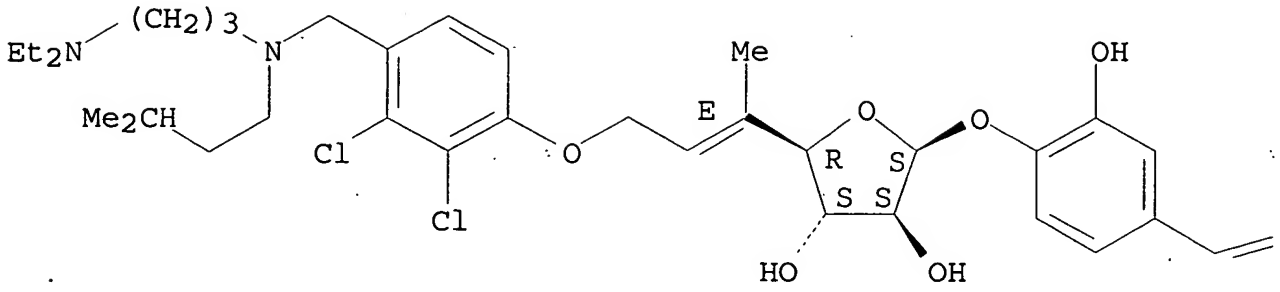
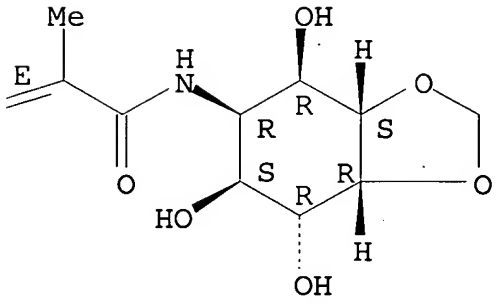
CN D-neo-Inositol, 5-deoxy-5-[[(2E)-3-[4-[[(5E)-5,6-dideoxy-7-O-[2,3-dichloro-4-[[[3-(diethylamino)propyl](3-methylbutyl)amino]methyl]phenyl]-5-methyl-β-D-arabino-hept-5-enofuranosyl]oxy]-3-hydroxyphenyl]-2-methyl-1-oxo-2-propenyl]amino]-1,2-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

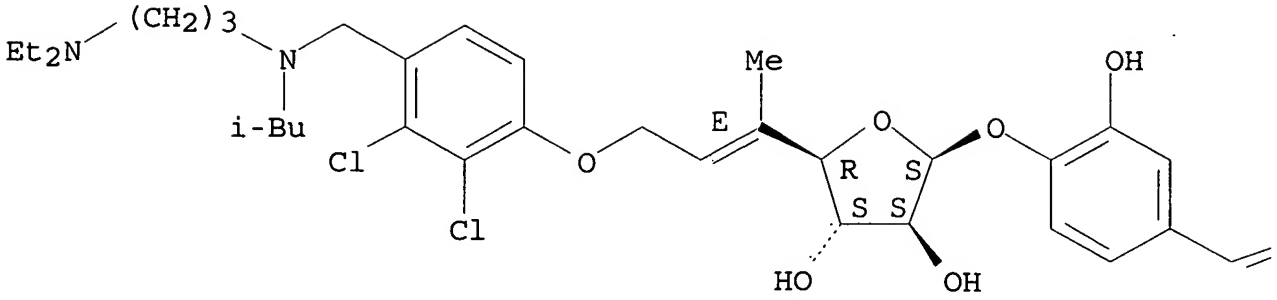


RN 377070-18-3 ZCA

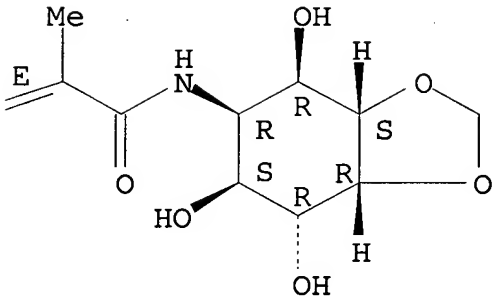
CN D-neo-Inositol, 5-deoxy-5-[[(2E)-3-[4-[[(5E)-5,6-dideoxy-7-O-[2,3-dichloro-4-[[[3-(diethylamino)propyl](2-methylpropyl)amino]methyl]phenyl]-5-methyl-β-D-arabino-hept-5-enofuranosyl]oxy]-3-hydroxyphenyl]-2-methyl-1-oxo-2-propenyl]amino]-1,2-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



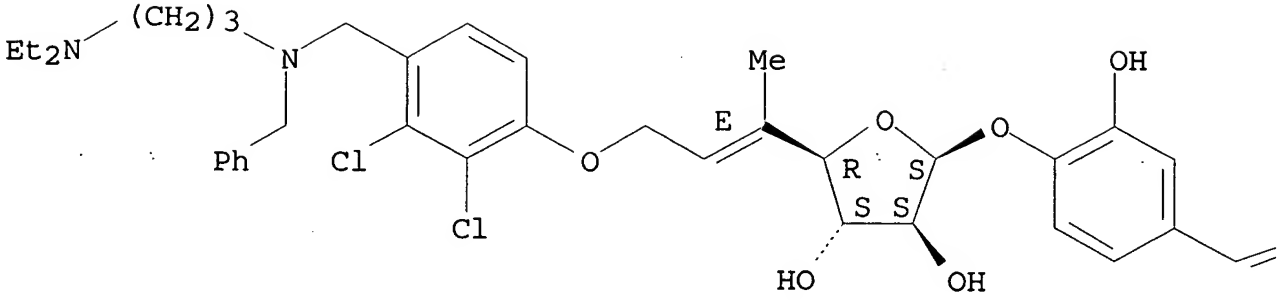
PAGE 1-B



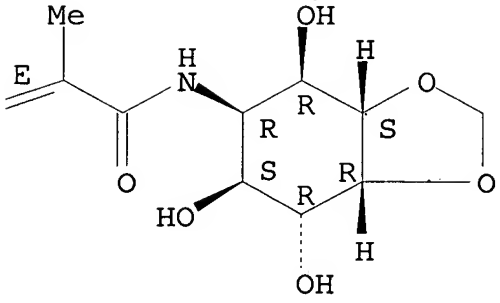
RN 377070-19-4 ZCA
CN D-neo-Inositol, 5-deoxy-5-[[(2E)-3-[4-[[(5E)-5,6-dideoxy-7-O-[2,3-dichloro-4-[[[3-(diethylamino)propyl](phenylmethyl)amino]methyl]phenyl]-5-methyl-β-D-arabino-hept-5-enofuranosyl]oxy]-3-hydroxyphenyl]-2-methyl-1-oxo-2-propenyl]amino]-1,2-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



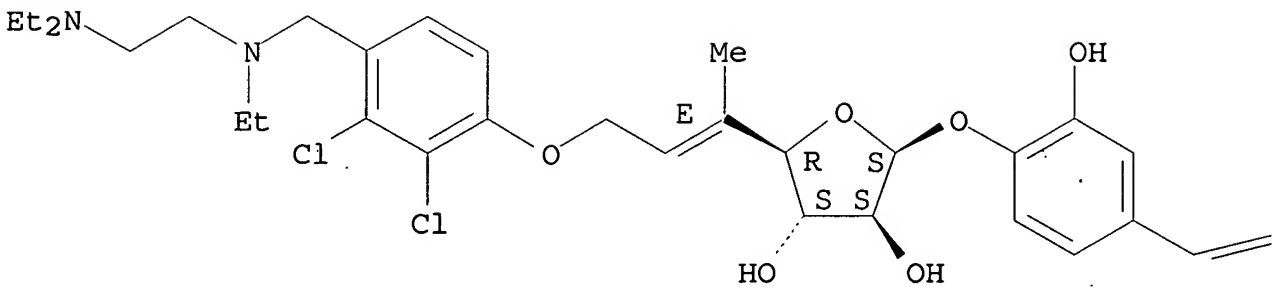
PAGE 1-B



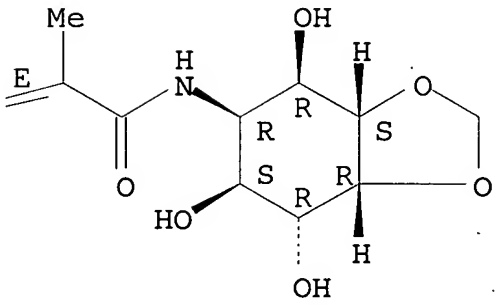
RN 377070-20-7 ZCA
CN D-neo-Inositol, 5-deoxy-5-[[(2E)-3-[4-[[(5E)-5,6-dideoxy-7-O-[2,3-dichloro-4-[[[2-(diethylamino)ethyl]ethylamino]methyl]phenyl]-5-methyl-β-D-arabino-hept-5-enofuranosyl]oxy]-3-hydroxyphenyl]-2-methyl-1-oxo-2-propenyl]amino]-1,2-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

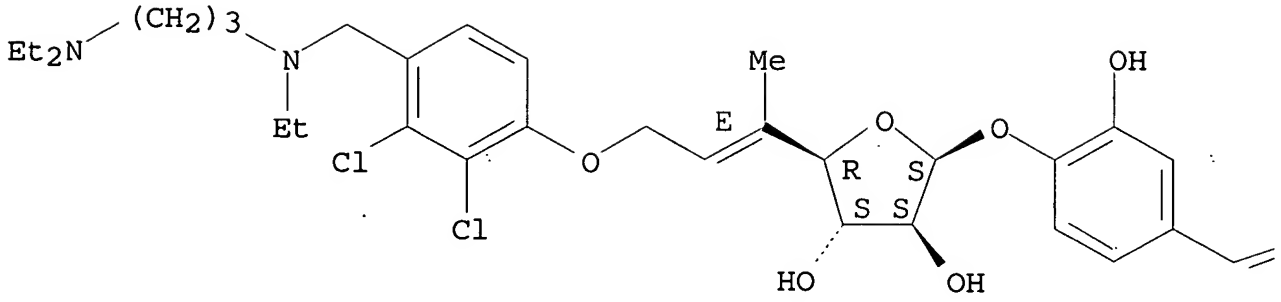


RN 377070-21-8 ZCA

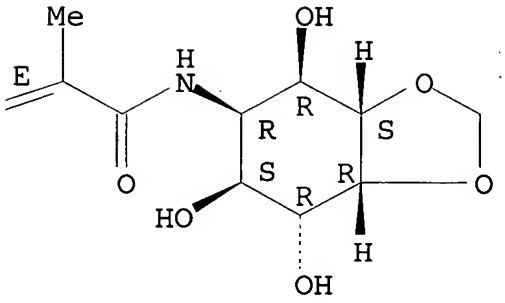
CN D-neo-Inositol, 5-deoxy-5-[[(2E)-3-[4-[[(5E)-5,6-dideoxy-7-O-[2,3-dichloro-4-[[[3-(diethylamino)propyl]ethylamino]methyl]phenyl]-5-methyl-β-D-arabino-hept-5-enofuranosyl]oxy]-3-hydroxyphenyl]-2-methyl-1-oxo-2-propenyl]amino]-1,2-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



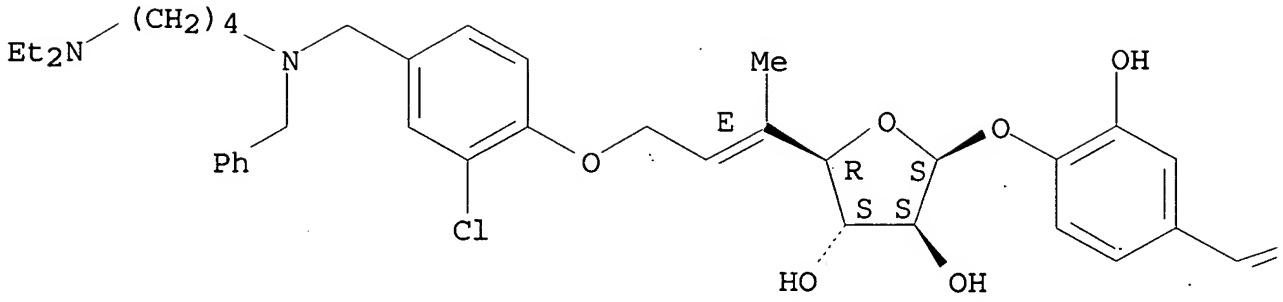
PAGE 1-B



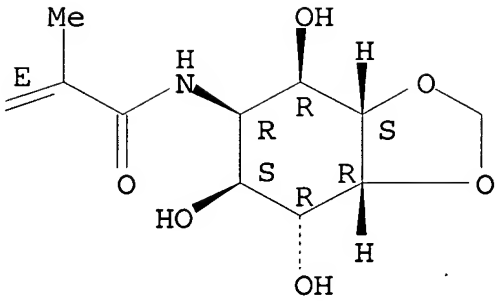
RN 377072-42-9 ZCA
CN D-neo-Inositol, 5-[[(2E)-3-[4-[[(5E)-7-O-[2-chloro-4-[[[4-[2-(diethylamino)ethyl]butyl](phenylmethyl)amino]methyl]phenyl]-5,6-dideoxy-5-methyl-β-D-arabino-hept-5-enofuranosyl]oxy]-3-hydroxyphenyl]-2-methyl-1-oxo-2-propenyl]amino]-5-deoxy-1,2-O-methylene- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



IT **377069-96-0P 377069-97-1P 377070-12-7P**
377070-13-8P 377070-14-9P 377070-15-0P
377070-16-1P 377070-17-2P 377070-18-3P
377070-19-4P 377070-20-7P 377070-21-8P
377072-42-9P
(prepn. of hygromycin A derivs. via Wittig reaction for the treatment of bacterial and protozoal infections)

L25 ANSWER 10 OF 22 ZCA COPYRIGHT 2007 ACS on STN
134:358891 Luminescence Energy Transfer with Lanthanide Chelates: Interpretation of Sensitized Acceptor Decay Amplitudes. Heyduk, Tomasz; Heyduk, Ewa (Edward A. Doisy Department of Biochemistry and Molecular Biology, St. Louis University Medical School, St. Louis, MO, 63104, USA). Analytical Biochemistry, 289(1), 60-67 (English) 2001. CODEN: ANBCA2. ISSN: 0003-2697. Publisher: Academic Press.

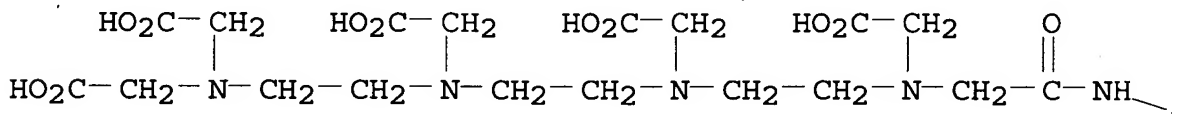
AB Lanthanide chelates used as donors offer several advantages over classical fluorescence probes in resonance energy transfer distance measurements. One of these advantages is that energy transfer can be conveniently measured using sensitized acceptor decay measurements. In these measurements a long μs lifetime of the lanthanide donor and a short ns lifetime of the acceptor allow elimination of a signal from the unquenched donor. The decay of sensitized acceptor emission reflects decay properties of the donor engaged in energy transfer. The amplitude of the sensitized acceptor signal is dependent on the resonance energy transfer rate const. In the case where there are ≥2 populations of donors with different energy transfer rate consts., the relative amplitudes of corresponding decay components obsd. in sensitized acceptor emission do not represent the relative populations of the donors. A minor population of donors with a high rate of energy transfer can produce sensitized acceptor decay which is dominated by a decay component corresponding to this minor donor population. Using a simple exptl. system of rapid diffusion limit energy transfer between a Eu chelate and Cy5 acceptor the predicted dependency of sensitized acceptor decay amplitude on the energy transfer rate is indeed obsd. Probably the relative importance of decay components obsd. in sensitized acceptor emission should be evaluated after an appropriate correction of their values such that they properly reflect possible different populations of donors. A method to perform such correction is described. (c) 2001 Academic Press.

IT **192372-66-0D**, europium complex
(luminescence energy transfer in relation to interpretation of sensitized acceptor decay amplitudes in Cy5)

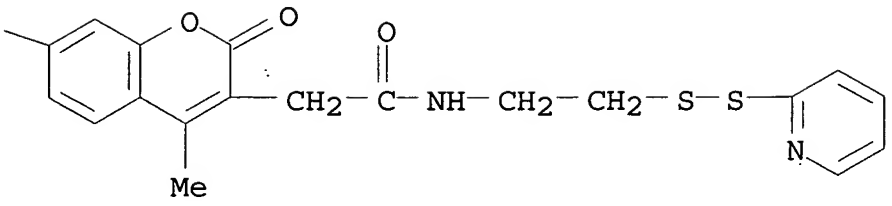
RN 192372-66-0 ZCA

CN 3,6,9,12-Tetraazatetradecanedioic acid, 3,6,9-tris(carboxymethyl)-12-[2-[[4-methyl-2-oxo-3-[2-oxo-2-[[2-(2-pyridinyldithio)ethyl]amino]ethyl]-2H-1-benzopyran-7-yl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



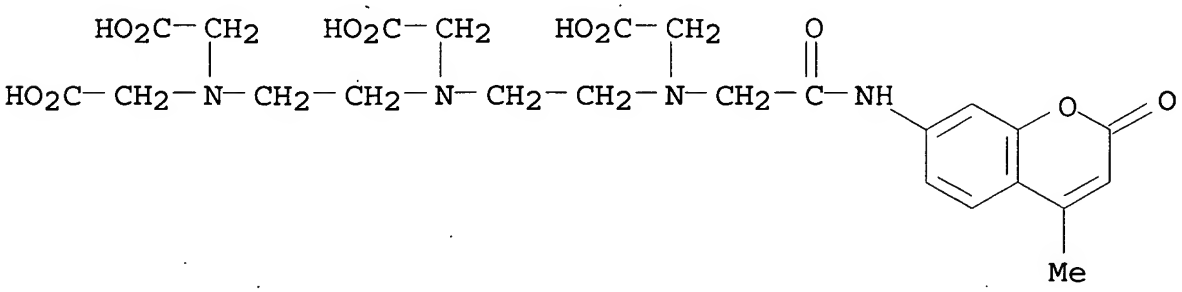
IT **192372-66-0D**, europium complex
(luminescence energy transfer in relation to interpretation of sensitized acceptor decay amplitudes in Cy5)

L25 ANSWER 11 OF 22 ZCA COPYRIGHT 2007 ACS on STN
132:354218 Sensitization of europium(III) luminescence by DTPA derivatives. Ozaki, Hiroaki; Suda, Emiko; Nagano, Toshihisa; Sawai, Hiroaki (Department of Chemistry, Faculty of Engineering, Gunma University, Gunma, 376-8515, Japan). Chemistry Letters (4), 312-313 (English) 2000. CODEN: CMLTAG. ISSN: 0366-7022. Publisher: Chemical Society of Japan.

AB Novel ligands, diethylenetriaminepentaacetic acid bearing several arom. amines, were synthesized and their chelates with a Eu ion were prepd. The lanthanide luminescence of the chelates of 1-aminonaphthalene and 7-amino-4-methylcoumarin was largely enhanced by the energy transfer from the ligand to the Eu ion.

IT **191661-03-7P 267649-00-3P**
(sensitization of europium(III) luminescence by DTPA derivs.)

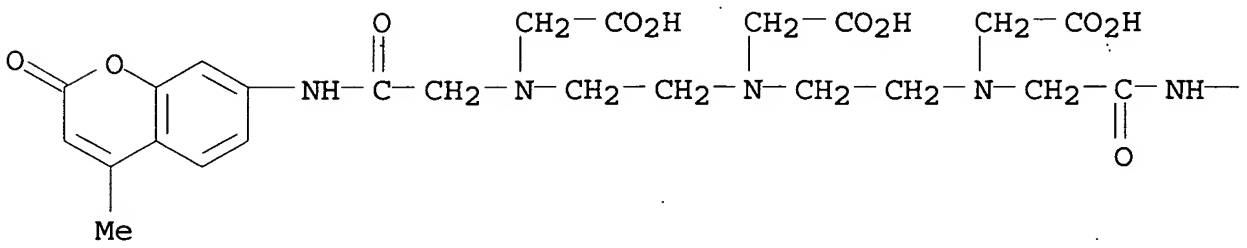
RN 191661-03-7 ZCA
CN Glycine, N-[2-[bis(carboxymethyl)amino]ethyl]-N-[2-[(carboxymethyl)[2-[(4-methyl-2-oxo-2H-1-benzopyran-7-yl)amino]-2-oxoethyl]amino]ethyl]- (9CI) (CA INDEX NAME)



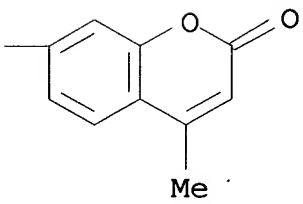
RN 267649-00-3 ZCA
CN Glycine, N,N-bis[2-[(carboxymethyl)[2-[(4-methyl-2-oxo-2H-1-

benzopyran-7-yl)amino]-2-oxoethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



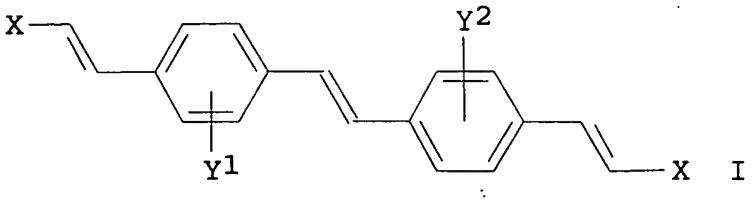
PAGE 1-B



IT **191661-03-7P 267649-00-3P**
(sensitization of europium(III) luminescence by DTPA derivs.)

L25 ANSWER 12 OF 22 ZCA COPYRIGHT 2007 ACS on STN
132:167676 Divinylstilbenesulfonic acid derivatives, their preparation and use. Eliu, Victor Paul; Rohringer, Peter; Volkel, Julia; Kramer, Hans (Ciba Specialty Chemicals Holding Inc., Switz.). PCT Int. Appl. WO 2000009471 A1 20000224, 31 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-EP5431 19990729. PRIORITY: EP 1998-810763 19980810.

GI



AB Stilbene derivs. I [X = CN, CO2R1, CONR2R3, C6H4R4; Y1, Y2 = H, SO3M; Y1 or Y2 = SO3M; M = H, alkali metal, alk. earth metal, amine; R1 = H, (un)substituted C1-18 alk(en)yl, C1-5 (poly)hydroxyalkyl, [O(CH2)n]mOH, amino, (un)substituted Ph; R2, R3 = H, (un)substituted C1-5 alkyl, (un)substituted Ph, or NR2R3 = 5- or 6-membered heterocyclyl; R4 = H, OH, CN, SO3H, halo, C1-5 alkyl, C1-5 alkoxy; m = 1-5; n = 1-3] are useful as fluorescent whiteners, esp. for detergents, paper, and cotton and synthetic polyamide fibers. Thus, 4,4'-diaminostilbene-2,2'-disulfonic acid was tetrazotized in HOAc, treated with NaHCO3, and condensed with Et acrylate in the presence of a Pd complex to give I (X = CO2Et, Y1 = Y2 = SO3Na) (II) in good yield. A 160 g/m2 paper sheet from 1:1 birch-pine kraft pulp (2.2% consistency) contg. 10% carbonate filler and 0.8% II showed ISO brightness 7.3, compared with 0.3 when II was omitted.

IT **259105-68-5P**
(divinylstilbenesulfonic acid derivs. as fluorescent whiteners)

RN 259105-68-5 ZCA

CN Benzenesulfonic acid, 2,2'-(1,2-ethenediyl)bis[5-[3-[[2-(diethylamino)ethyl]amino]-3-oxo-1-propenyl]-, disodium salt (9CI) (CA INDEX NAME)

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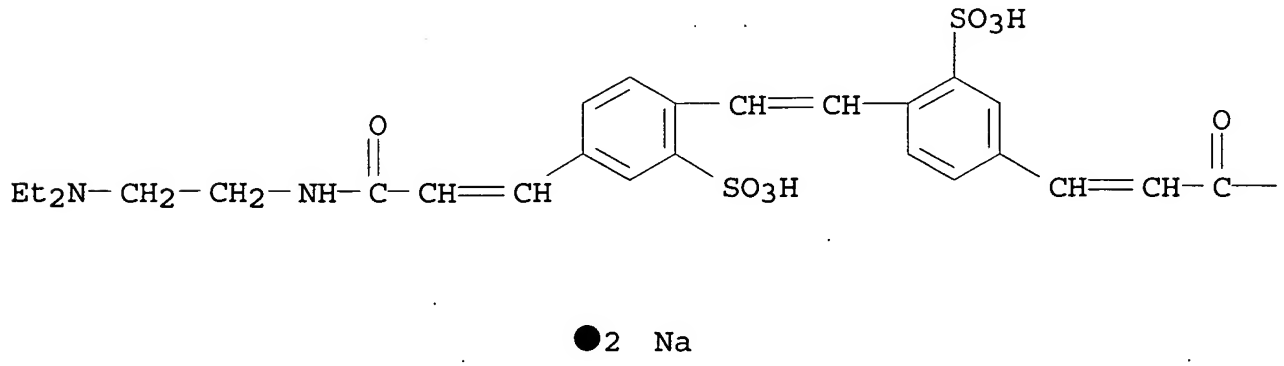
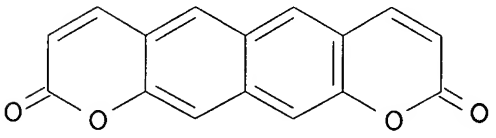


PAGE 1-B

—NH—CH_2—CH_2—NEt_2

IT **259105-68-5P**
(divinylstilbenesulfonic acid derivs. as fluorescent whiteners)

L25 ANSWER 13 OF 22 ZCA COPYRIGHT 2007 ACS on STN
131:18938 Synthesis of 2H,9H-naphtho[2,3-b:7,6-b']dipyran-2,9-diones as potential DNA-reactive agents. Zagotto, Giuseppe; Palumbo, Manlio; Uriarte, Eugenio; Bonsignore, Leonardo; Delogu, Giovanna; Podda, Gianni (Department of Pharmaceutical Sciences, University of Padua, Padua, 35131, Italy). Farmaco, 53(10,11), 675-679 (English) 1998. CODEN: FRMCE8. ISSN: 0014-827X. Publisher: Elsevier Science S.A..
GI



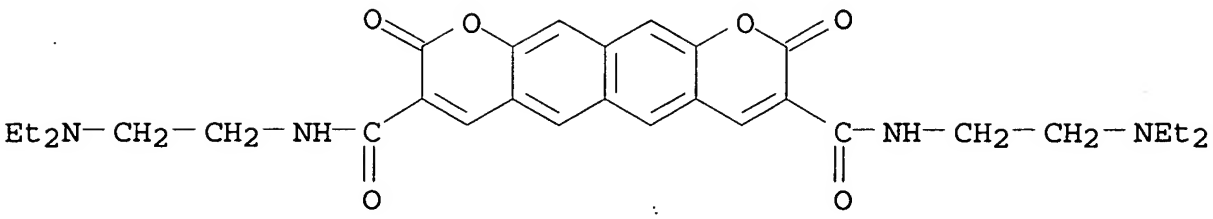
I

AB A new 2H,9H-naphtho[2,3-b:7,6-b']dipyran-2,9-dione I has been synthesized. The tetracyclic deriv. was obtained by two different synthetic pathways, both having, as a common intermediate, the 3,6-dihydroxynaphthalene-2,7-dicarboxaldehyde (II). Thus, II reacted with EtOCCH2CN to give a tetracyclic acid which was decarboxylated to I. I was also prepd. via amide and ester derivs. of II.

IT **226561-46-2P**
(prepn. of naphthodipyrandione)

RN 226561-46-2 ZCA

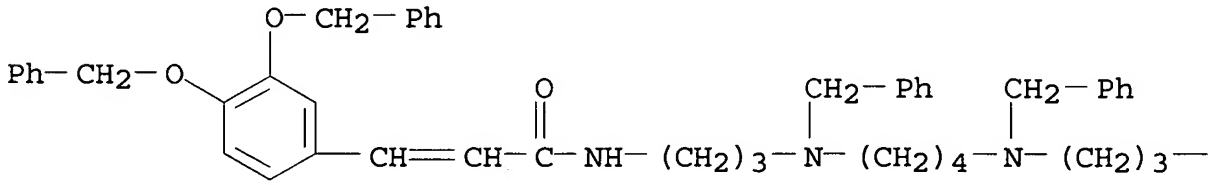
CN 2H,9H-Naphtho[2,3-b:7,6-b']dipyran-3,8-dicarboxamide, N,N'-bis[2-(diethylamino)ethyl]-2,9-dioxo- (9CI) (CA INDEX NAME)



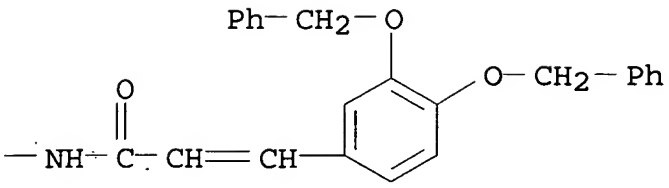
IT **226561-46-2P**
(prepn. of naphthodipyrandione)

L25 ANSWER 14 OF 22 ZCA COPYRIGHT 2007 ACS on STN
129:189515 Simple fragment syntheses of all four isomers of the spermine alkaloid kukoamine. Karigiannis, George; Mamos, Petros; Balayiannis, George; Katsoulis, Ioannis; Papaioannou, Dionissios (Department of Chemistry, University of Patras, Patras, 265 00, Greece). Tetrahedron Letters, 39(28), 5117-5120 (English) 1998. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd.,
AB All four isomers of the spermine alkaloid kukoamine were unambiguously prepd. through diacylation with O,O'-dibenzylcaffeyl chloride of suitably protected (benzyl and/or trityl groups) spermine derivs., assembled on solid and/or in liq. phase using β-alanine and γ-aminobutyric acid, followed by simultaneous N- and O- deprotection and double bond redn. using catalytic hydrogenation.
IT **211632-77-8P**
(fragment syntheses of all four isomers of spermine alkaloid kukoamine)
RN 211632-77-8 ZCA
CN 2-Propenamide, N,N'-[1,4-butanediylbis[[(phenylmethyl)imino]-3,1-propanediyl]]bis[3,4-bis(phenylmethoxy)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



IT **211632-77-8P**
(fragment syntheses of all four isomers of spermine alkaloid kukoamine)

L25 ANSWER 15 OF 22 ZCA COPYRIGHT 2007 ACS on STN
127:106264 Thiol-reactive, luminescent europium chelates: luminescence probes for resonance energy transfer distance measurements in biomolecules. Heyduk, Ewa; Heyduk, Tomasz (Edward A. Doisy Department of Biochemistry and Molecular Biology, St. Louis University Medical School, St. Louis, MO, 63104, USA). Analytical Biochemistry, 248(2), 216-227 (English) 1997. CODEN: ANBCA2. ISSN: 0003-2697. Publisher: Academic.

AB Lanthanide chelates have recently been shown to be extremely promising luminescence probes for distance measurements in biomols. using luminescence resonance energy transfer measurements. The authors describe simple procedures for prepg. highly fluorescent thiol-reactive europium chelates. These new compds. contain a UV-absorbing coumarin group which sensitizes europium emission, diethylenetriaminepentaacetic acid or triethylenetetraaminehexaaceti c acid groups which provide europium chelating function, and a pyridyl disulfide group which allows specific modification of thiol groups. These reagents can be used to label proteins at Cys residues or synthetic oligonucleotides which contain thiol groups. Modification can be reversed easily by treatment with a reducing agent (dithiothreitol). Luminescence energy transfer between these new chelates and CY5 fluorochrome attached to the opposite ends of 15-bp double-stranded DNA was measured to test their usefulness for distance measurements in macromols. The distance measured between the chelate (donor) and CY5 (acceptor) was in the range expected for the length of 15-bp DNA. The stability of europium chelates and their conjugates with a protein, the precision of distance measurements using these chelates, possible errors due to intramol. energy transfer, and the modulation of the R0 value with deuterium oxide were tested. The results obtained fully confirmed the great potential of these new probes for sensitive, simple, and precise distance measurements in biomols. using luminescence resonance energy transfer.

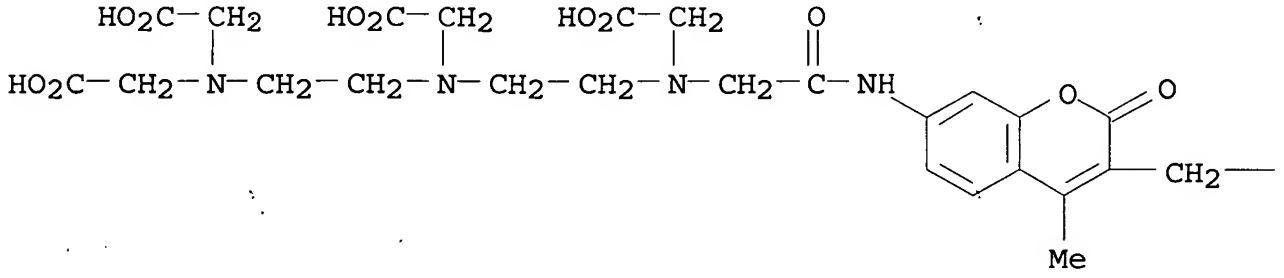
IT **192372-65-9DP**, europium complexes **192372-66-0DP**,

europium complexes **192372-67-1DP**, europium complexes **192372-68-2DP**, europium complexes
(thiol-reactive europium chelates as luminescence probes for resonance energy transfer in biomols.)

RN 192372-65-9 ZCA

CN Glycine, N-[2-[bis(carboxymethyl)amino]ethyl]-N-[2-[(carboxymethyl)[2-[[4-methyl-2-oxo-3-[2-oxo-2-[[2-(2-pyridinyldithio)ethyl]amino]ethyl]-2H-1-benzopyran-7-yl]amino]-2-oxoethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



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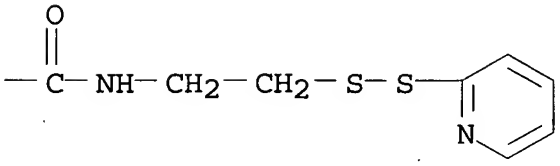

RN 192372-66-0 ZCA

CN 3,6,9,12-Tetraazatetradecanedioic acid, 3,6,9-tris(carboxymethyl)-12-[2-[[4-methyl-2-oxo-3-[2-oxo-2-[[2-(2-pyridinyldithio)ethyl]amino]ethyl]-2H-1-benzopyran-7-yl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

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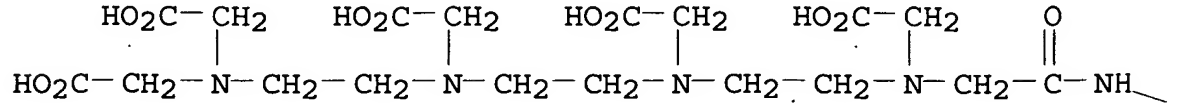
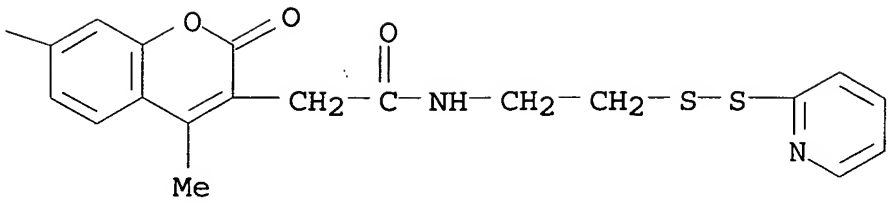
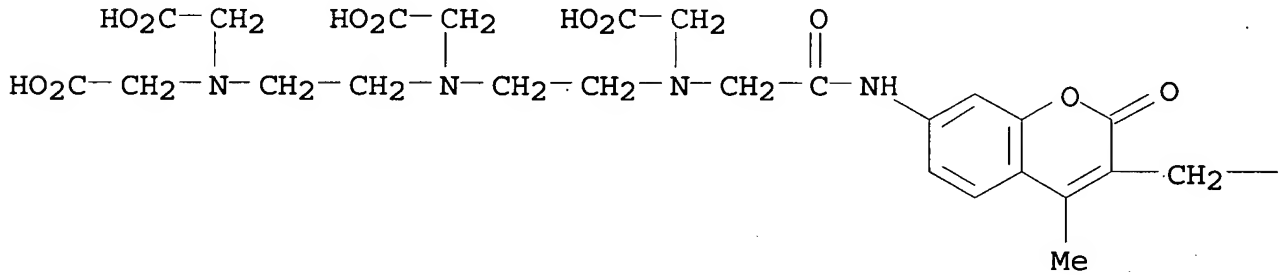


PAGE 1-B

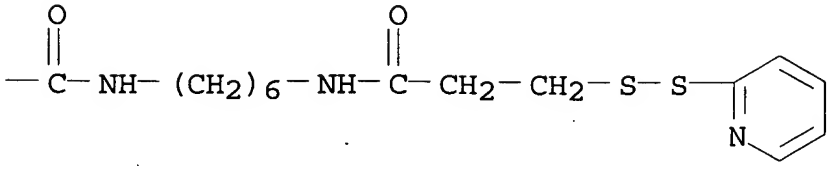


RN 192372-67-1 ZCA
CN Glycine, N-[2-[bis(carboxymethyl)amino]ethyl]-N-[2-[(carboxymethyl)[2-[[4-methyl-2-oxo-3-[2-oxo-2-[[6-[[1-oxo-3-(2-pyridinyldithio)propyl]amino]hexyl]amino]ethyl]-2H-1-benzopyran-7-yl]amino]-2-oxoethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



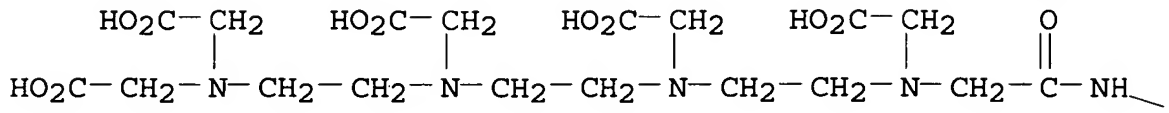
PAGE 1-B



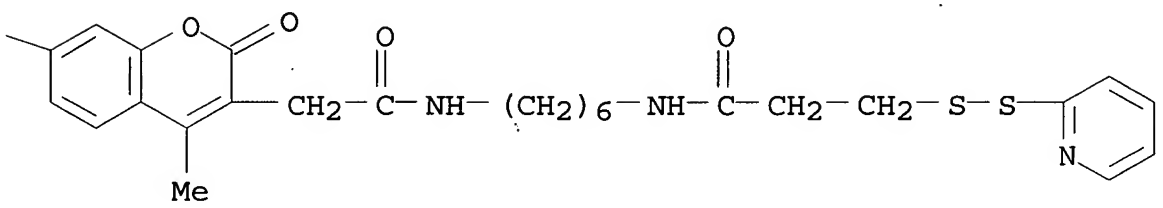
RN 192372-68-2 ZCA
CN 3,6,9,12-Tetraazatetradecanedioic acid, 3,6,9-tris(carboxymethyl)-12-[2-[[4-methyl-2-oxo-3-[2-oxo-2-[[6-[[1-oxo-3-(2-pyridinyldithio)propyl]amino]hexyl]amino]ethyl]-2H-1-benzopyran-7-

yl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

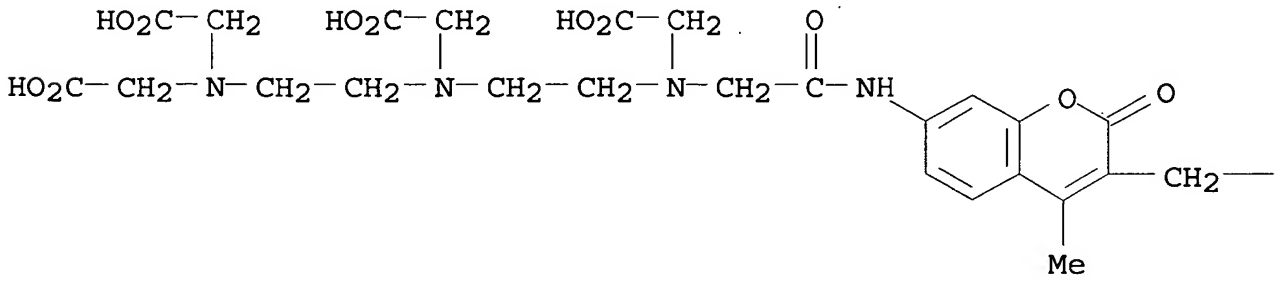


IT **192372-65-9P 192372-66-0P 192372-67-1P**
192372-68-2P
(thiol-reactive europium chelates as luminescence probes for resonance energy transfer in biomols.)

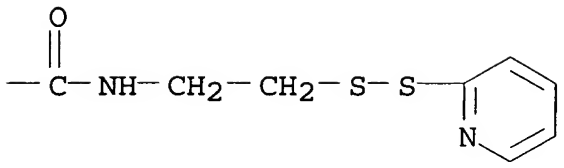
RN 192372-65-9 ZCA

CN Glycine, N-[2-[bis(carboxymethyl)amino]ethyl]-N-[2-[(carboxymethyl)[2-[[4-methyl-2-oxo-3-[2-oxo-2-[[2-(2-pyridinyldithio)ethyl]amino]ethyl]-2H-1-benzopyran-7-yl]amino]-2-oxoethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

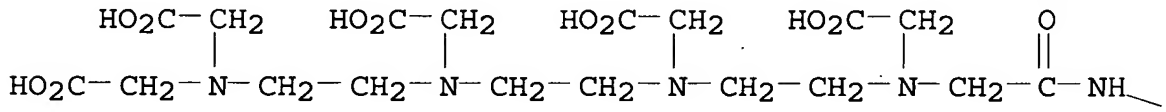


PAGE 1-B

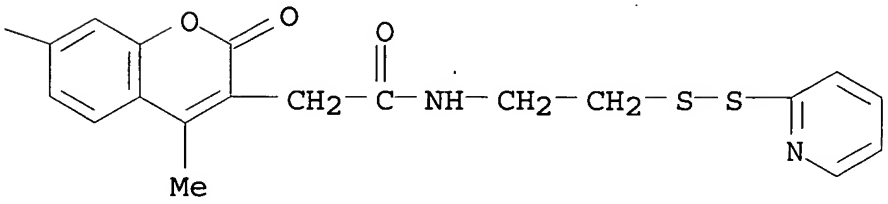


RN 192372-66-0 ZCA
CN 3,6,9,12-Tetraazatetradecanedioic acid, 3,6,9-tris(carboxymethyl)-12-[2-[[4-methyl-2-oxo-3-[2-oxo-2-[[2-(2-pyridinyldithio)ethyl]amino]ethyl]-2H-1-benzopyran-7-yl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

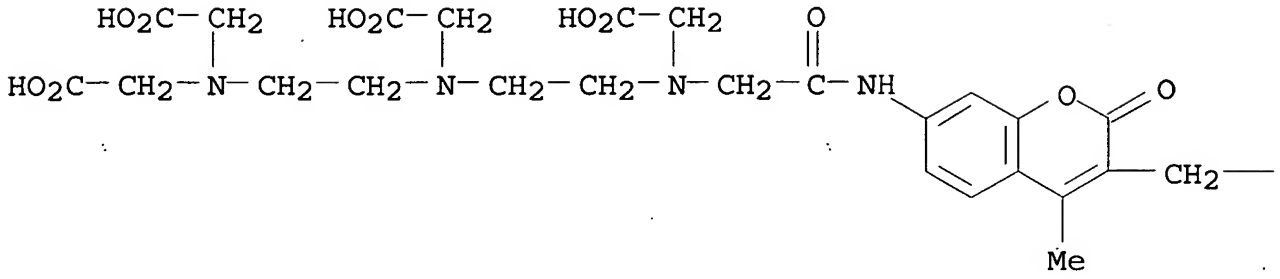


PAGE 1-B

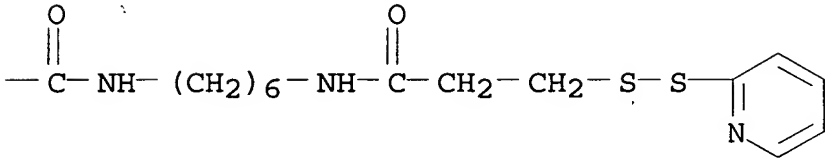


RN 192372-67-1 ZCA
CN Glycine, N-[2-[bis(carboxymethyl)amino]ethyl]-N-[2-[(carboxymethyl)[2-[[4-methyl-2-oxo-3-[2-oxo-2-[[6-[[1-oxo-3-(2-pyridinyldithio)propyl]amino]hexyl]amino]ethyl]-2H-1-benzopyran-7-yl]amino]-2-oxoethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

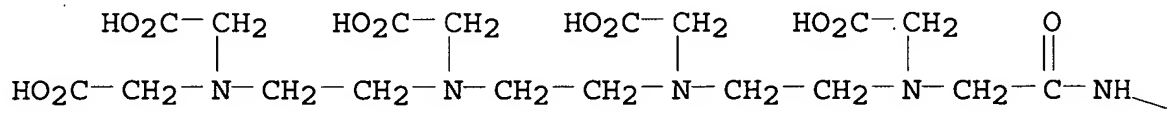


PAGE 1-B

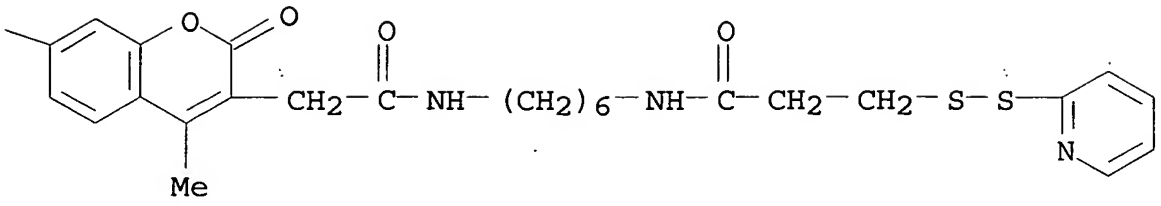


RN 192372-68-2 ZCA
CN 3,6,9,12-Tetraazatetradecanedioic acid, 3,6,9-tris(carboxymethyl)-12-[2-[[4-methyl-2-oxo-3-[2-oxo-2-[[6-[[1-oxo-3-(2-pyridinyldithio)propyl]amino]hexyl]amino]ethyl]-2H-1-benzopyran-7-yl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



IT **192372-65-9DP**, europium complexes **192372-66-0DP**, europium complexes **192372-67-1DP**, europium complexes **192372-68-2DP**, europium complexes
(thiol-reactive europium chelates as luminescence probes for resonance energy transfer in biomols.)

IT **192372-65-9P 192372-66-0P 192372-67-1P 192372-68-2P**
(thiol-reactive europium chelates as luminescence probes for resonance energy transfer in biomols.)

L25 ANSWER 16 OF 22 ZCA COPYRIGHT 2007 ACS on STN

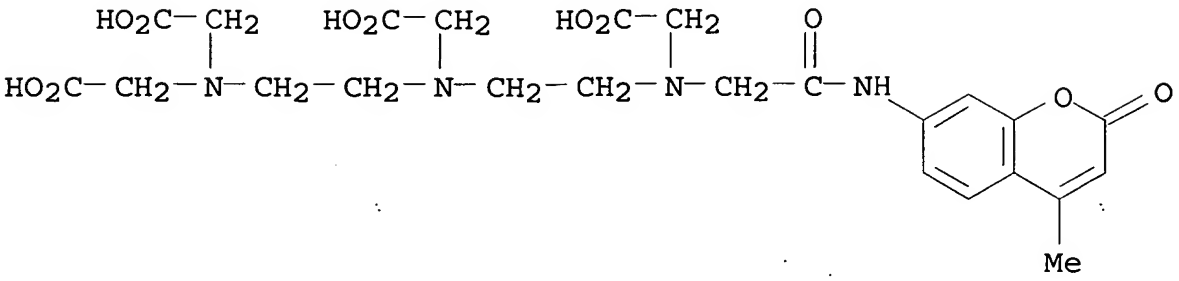
127:77478 Immobilization of lanthanide ion chelates on DNA and their luminescence properties. Ozaki, H.; Matsuzawa, N.; Suda, E.; Sawai, H. (Department Chemistry, Gunma University, Gunma, 376, Japan). Kidorui, 30, 358-359 (Japanese) 1997. CODEN: KIDOEP. ISSN: 0910-2205. Publisher: Nippon Kidorui Gakkai.

AB EDTA derivs. were synthesized as the ligands for the chelating lanthanide ion and their europium chelate were immobilized on DNA at an appropriate site. The fluorescence spectra of the Eu3+-chelate-labeled DNAs show the enhanced luminescence of europium. In addn., several kind of arom. compd.-attached DTPA derivs. were synthesized and the sensitizing effect of fluorescence were investigated.

IT **191661-03-7P**
(immobilization of lanthanide ion chelates on DNA and their luminescence properties)

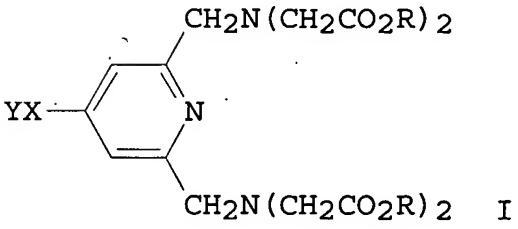
RN 191661-03-7 ZCA

CN Glycine, N-[2-[bis(carboxymethyl)amino]ethyl]-N-[2-[(carboxymethyl)[2-[(4-methyl-2-oxo-2H-1-benzopyran-7-yl)amino]-2-oxoethyl]amino]ethyl]- (9CI) (CA INDEX NAME)



IT **191661-03-7P**
(immobilization of lanthanide ion chelates on DNA and their luminescence properties)

L25 ANSWER 17 OF 22 ZCA COPYRIGHT 2007 ACS on STN
120:158200 Photochemical labeling of nucleic acids with europium-chelating reagents and their use in gene probe systems. Loebberding, Antonius; Mikhail, Gamal K.; Springer, Wolfgang; Hugl, Herbert; Koecher, Juergen (Bayer A.-G., Germany). Eur. Pat. Appl. EP 578067 A1 19940112, 15 pp. DESIGNATED STATES: R: CH, DE, FR, GB, IT, LI, NL, SE. (German). CODEN: EPXXDW. APPLICATION: EP 1993-110109 19930624. PRIORITY: DE 1992-4222255 19920707.
GI



AB A lanthanide-chelating structure I [X = (optionally hetero atom-contg.) alkylene or arylene; Y (or X + Y) = N-oxysuccinimido, N-maleimido, NH2, OH, halo, haloacetyl, etc.; R = H, alkali or alk. earth metal, ammonium] is coupled via a spacer (e.g. polyalkylamine, PEG) with a furocoumarin deriv. (e.g. angelicin or psoralen deriv.) for use as a photochem. labeling reagent, esp. for nucleic acid probes. Thus, 2,6-bis[N,N-bis(tert-butoxycarbonylmethyl)aminomethyl]-4-bromopyridine was condensed with 1-undecyn-10-ol with a Pd catalyst and the product was hydrogenated over PdO2, activated with carbonyldiimidazole, and reacted with N1-(angelicinamido)-N4,N9-

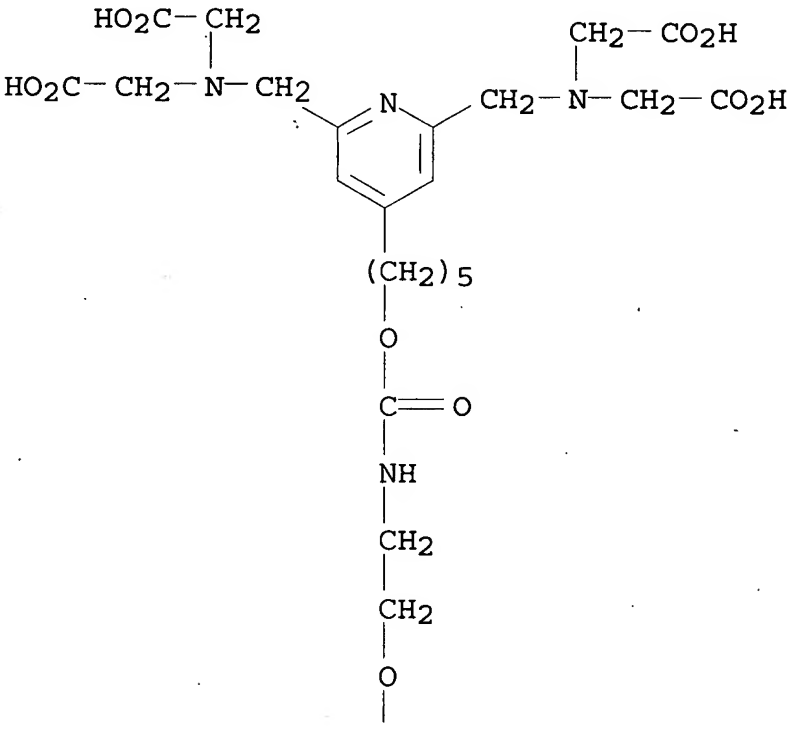
dimethylspermine (prepn. given) to produce a I which was used to photolabel DNA.

IT **153235-24-6P 153235-25-7P 153235-27-9P**
(prepn. and chelation with lanthanides, for photochem. labeling of nucleic acid probes)

RN 153235-24-6 ZCA

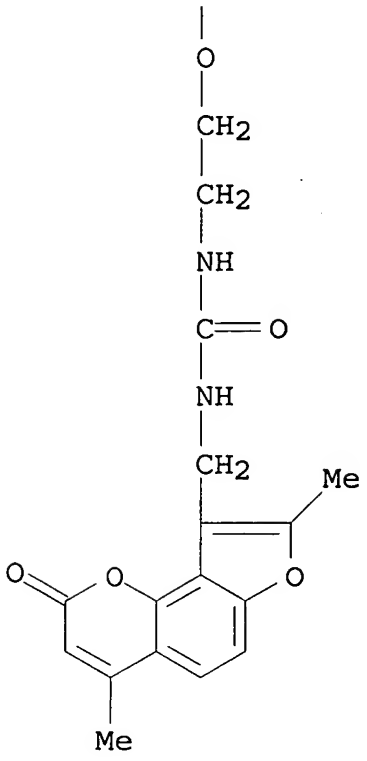
CN 7,10,13,16,19-Pentaoxa-2,4,22-triazatricosan-23-oic acid, 1-(4,8-dimethyl-2-oxo-2H-furo[2,3-h]-1-benzopyran-9-yl)-3-oxo-, 5-[2,6-bis[[bis(carboxymethyl)amino]methyl]-4-pyridinyl]pentyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



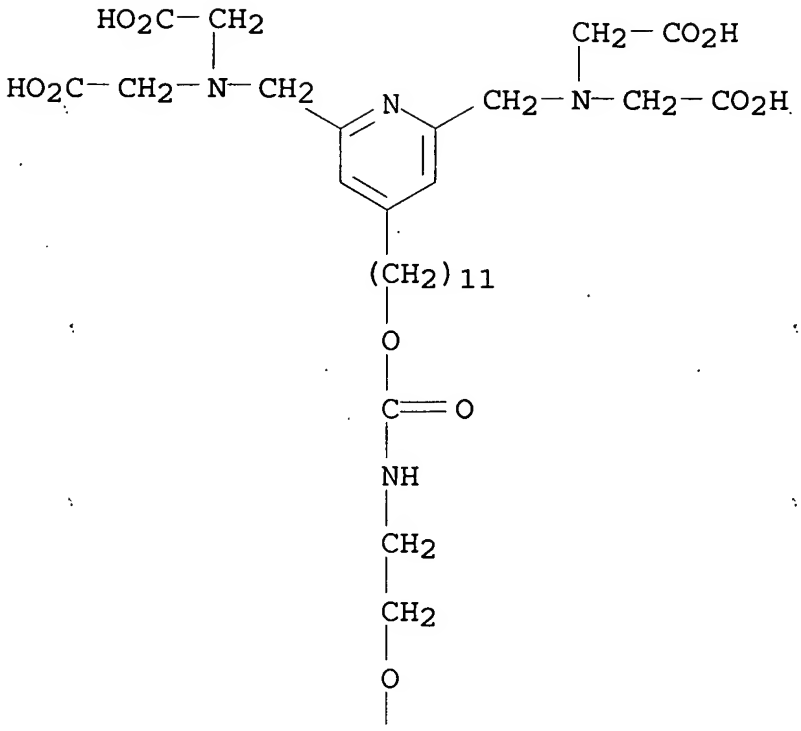
PAGE 2-A

PAGE 3-A

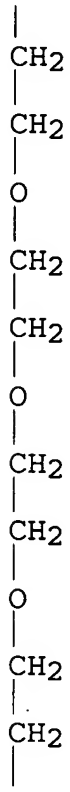


RN 153235-25-7 ZCA
CN 7,10,13,16,19-Pentaoxa-2,4,22-triazatricosan-23-oic acid, 1-(4,8-dimethyl-2-oxo-2H-furo[2,3-h]-1-benzopyran-9-yl)-3-oxo-, 11-[2,6-bis[[bis(carboxymethyl)amino]methyl]-4-pyridinyl]undecyl ester (9CI) (CA INDEX NAME)

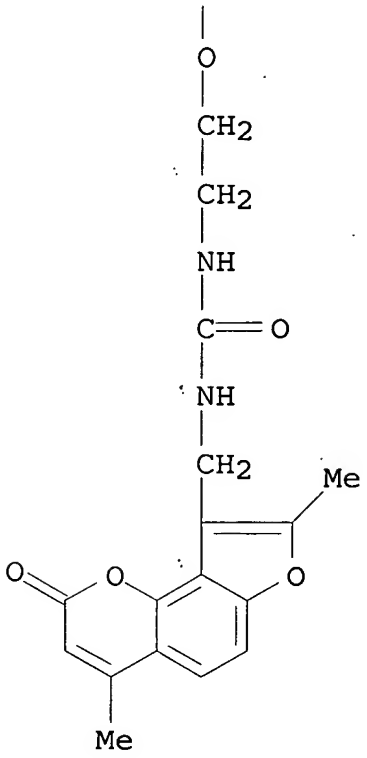
PAGE 1-A


HO2C— CH2
HO2C— CH2— N— CH2
CH2— CO2H
CH2— N— CH2— CO2H
N
(CH2)11
O
C═O
NH
CH2
CH2
O

PAGE 2-A

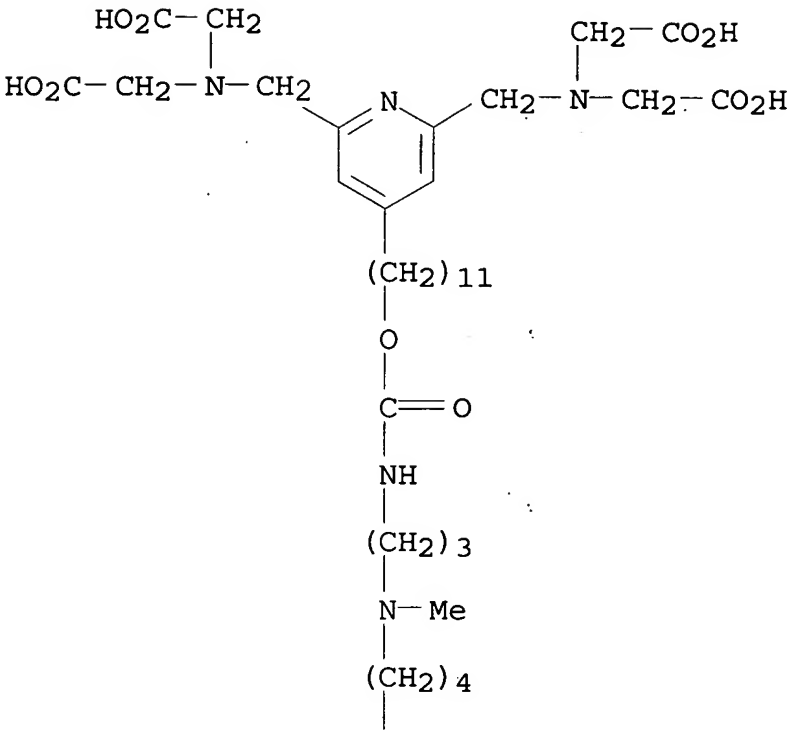


PAGE 3-A

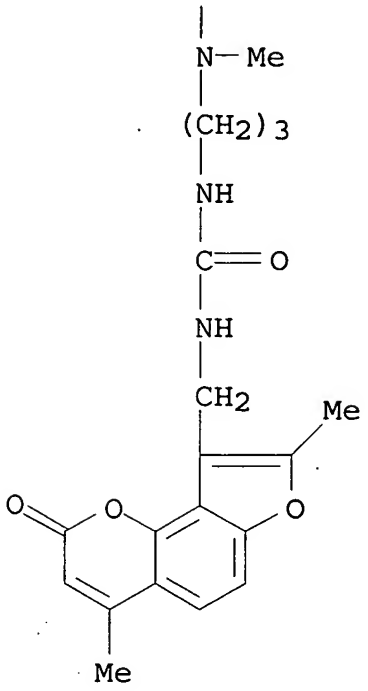


RN 153235-27-9 ZCA
CN 2,4,8,13,17-Pentaazaoctadecan-18-oic acid, 1-(4,8-dimethyl-2-oxo-2H-furo[2,3-h]-1-benzopyran-9-yl)-8,13-dimethyl-3-oxo-, 11-[2,6-bis[[bis(carboxymethyl)amino]methyl]-4-pyridinyl]undecyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

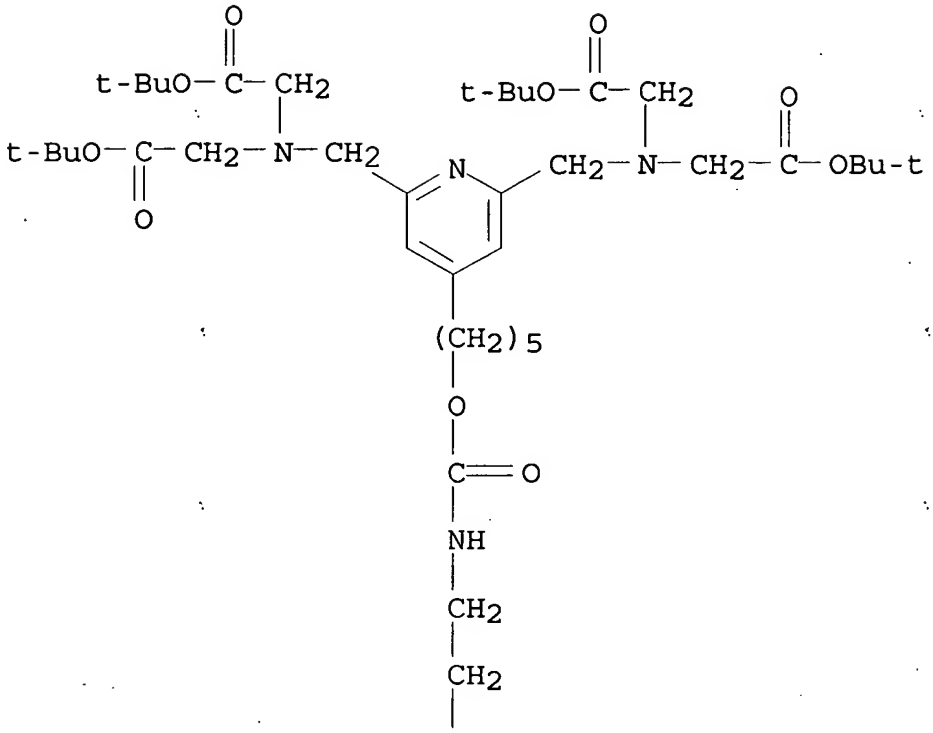

HO2C— CH2
HO2C— CH2— N— CH2
N
CH2— CO2H
CH2— N— CH2— CO2H
(CH2)11
O
C═O
NH
(CH2)3
N— Me
(CH2)4

PAGE 2-A



IT **153235-22-4P 153235-23-5P 153235-28-0P**
(prepn. and hydrolysis of)
RN 153235-22-4 ZCA
CN 7,10,13,16,19-Pentaoxa-2,4,22-triazatricosan-23-oic acid, 1-(4,8-dimethyl-2-oxo-2H-furo[2,3-h]-1-benzopyran-9-yl)-3-oxo-, 5-[2,6-bis[[bis[2-(1,1-dimethylethoxy)-2-oxoethyl]amino]methyl]-4-pyridinyl]pentyl ester (9CI) (CA INDEX NAME)

PAGE 1-A


t-BuO
C
CH2
t-BuO
C
CH2
N
CH2
O
t-BuO
C
CH2
CH2
N
CH2
C
OBu-t
O
N
(CH2)5
O
C
O
NH
CH2
CH2

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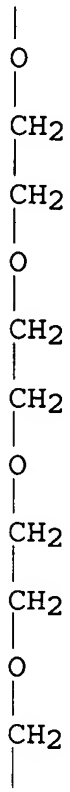
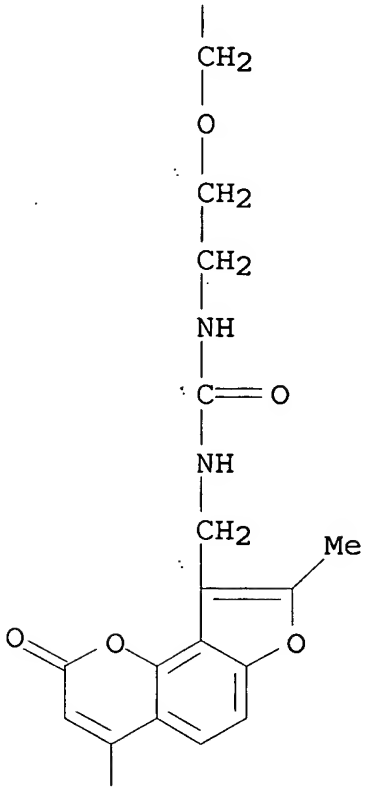


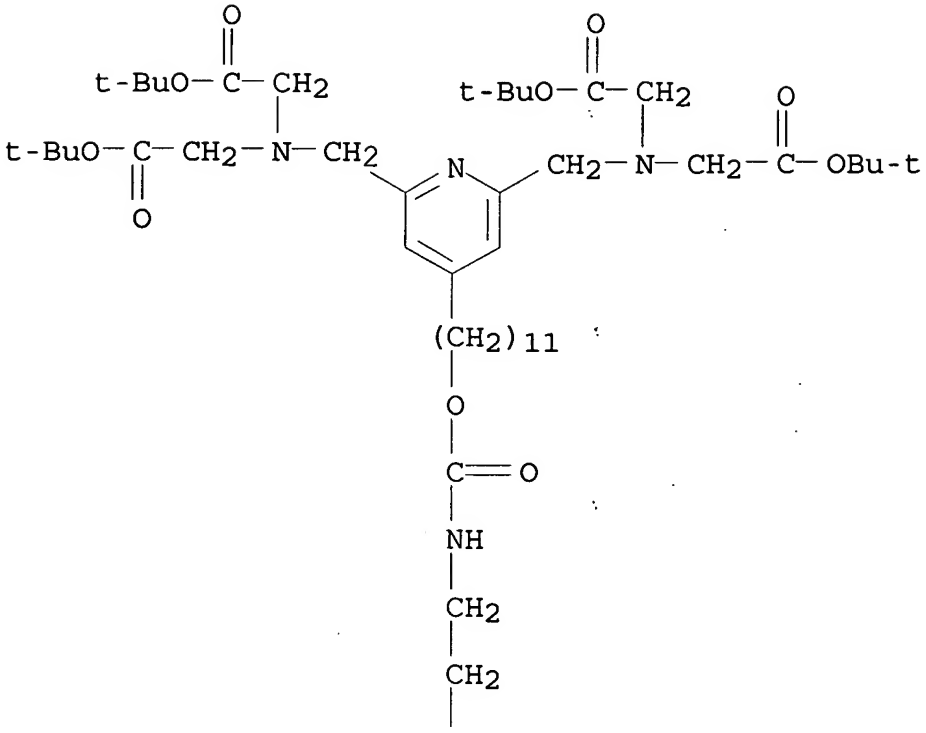
PAGE 3-A



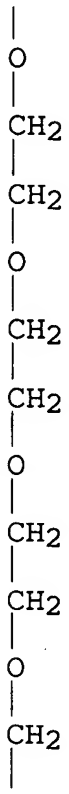
PAGE 4-A

RN 153235-23-5 ZCA
CN 7,10,13,16,19-Pentaoxa-2,4,22-triazatricosan-23-oic acid, 1-(4,8-dimethyl-2-oxo-2H-furo[2,3-h]-1-benzopyran-9-yl)-3-oxo-, 11-[2,6-bis[[bis[2-(1,1-dimethylethoxy)-2-oxoethyl]amino]methyl]-4-pyridinyl]undecyl ester (9CI) (CA INDEX NAME)

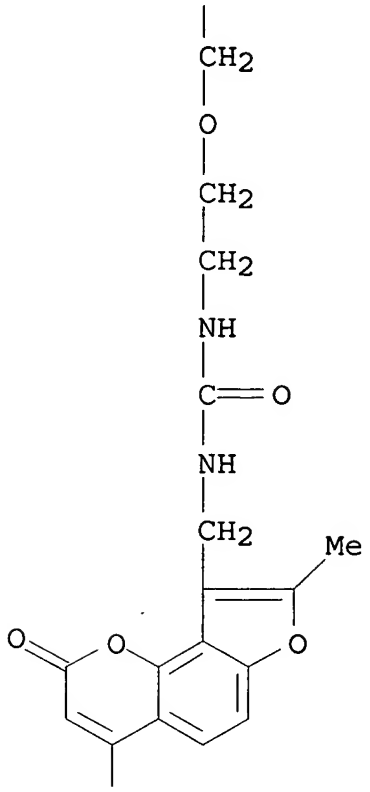
PAGE 1-A



PAGE 2-A



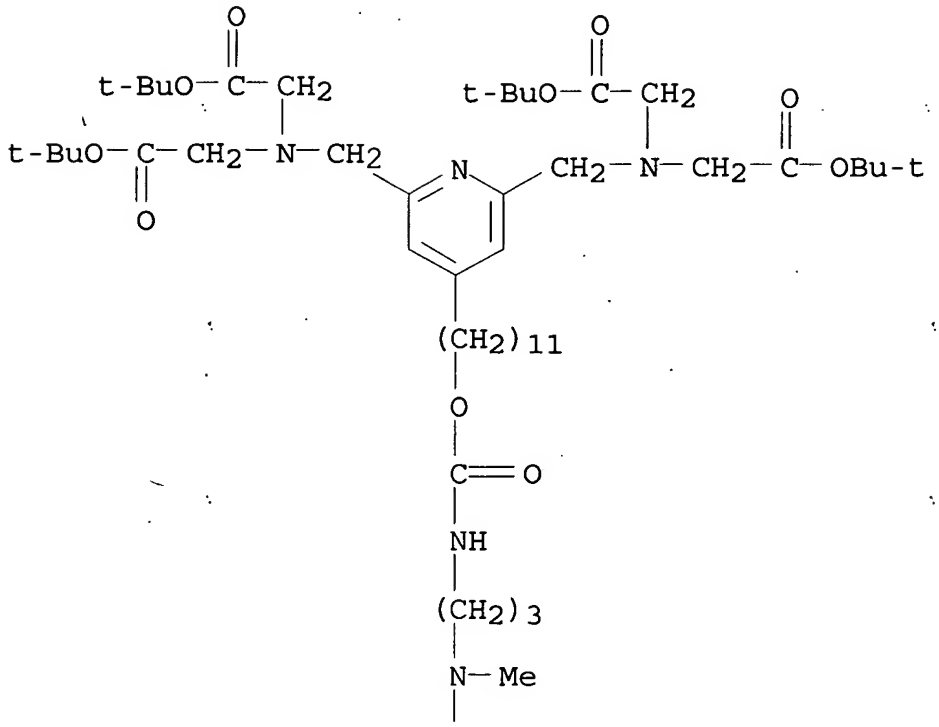
PAGE 3-A



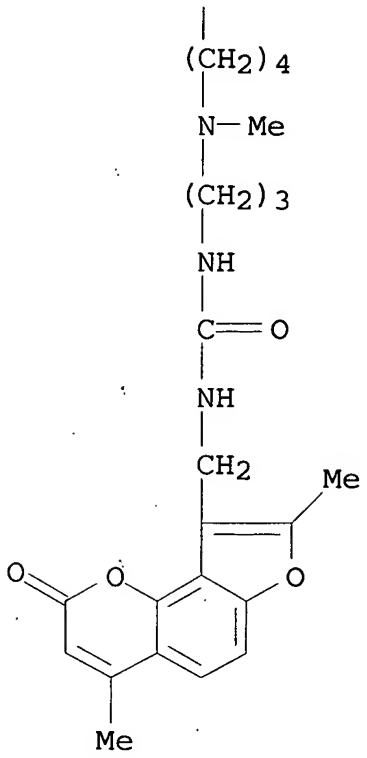
PAGE 4-A

RN 153235-28-0 ZCA
CN 2,4,8,13,17-Pentaazaoctadecan-18-oic acid, 1-(4,8-dimethyl-2-oxo-2H-furo[2,3-h]-1-benzopyran-9-yl)-8,13-dimethyl-3-oxo-, 11-[2,6-bis[[bis[2-(1,1-dimethylethoxy)-2-oxoethyl]amino]methyl]-4-pyridinyl]undecyl ester (9CI) (CA INDEX NAME)

PAGE 1-A


t-BuO
C
CH2
t-BuO
C
CH2
N
CH2
t-BuO
C
CH2
N
CH2
C
OBu-t
O
O
O
O
O
N
(CH2)11
O
C
O
NH
(CH2)3
N
Me

PAGE 2-A



IT **153235-24-6P 153235-25-7P 153235-27-9P**
(prepn. and chelation with lanthanides, for photochem. labeling of nucleic acid probes)

IT **153235-22-4P 153235-23-5P 153235-28-0P**
(prepn. and hydrolysis of)

L25 ANSWER 18 OF 22 ZCA COPYRIGHT 2007 ACS on STN

119:159802 Synthesis and antiallergic activity in the series of cinnamic acid derivatives. Saraf, A. S.; Simonyan, A. V. (Pyatigorsk. Farm. Inst., Russia). Khimiko-Farmatsevticheskii Zhurnal, 26(7-8), 45-8 (Russian) 1992. CODEN: KHFZAN. ISSN: 0023-1134.

AB The paper provides the rationale for the antiallergic activity of cinnamic acid derivs. and coumarin. There has been prediction and subsequent goal-oriented synthesis of new series of cinnamic acid derivs. The mechanisms of their structure-antiallergic activity relationships have been found. It is suggested that this type of the activity shown by coumarins is due to their potential conversion to cinnamic acids in the body as a result of decyclization.

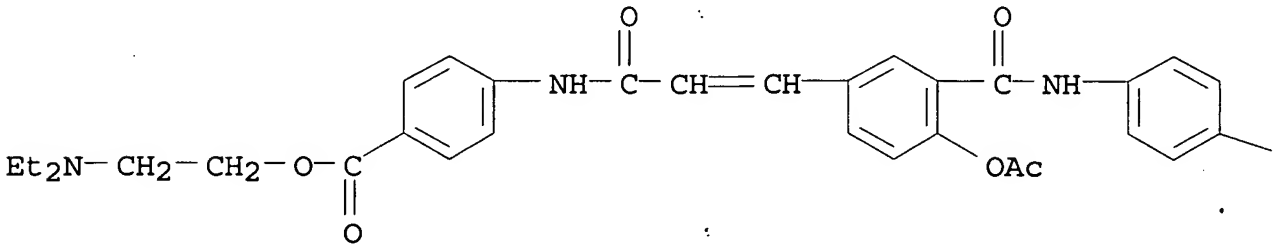
IT **150231-93-9P 150253-46-6P**
(prepn. of, as allergy inhibitor)

RN 150231-93-9 ZCA

CN Benzoic acid, 4-[[3-[4-(acetyloxy)-3-[[[4-[[2-

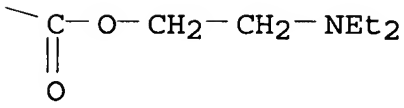
(diethylamino)ethoxy]carbonyl]phenyl]amino]carbonyl]phenyl]-1-oxo-2-propenyl]amino]-, 2-(diethylamino)ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



●2 HCl

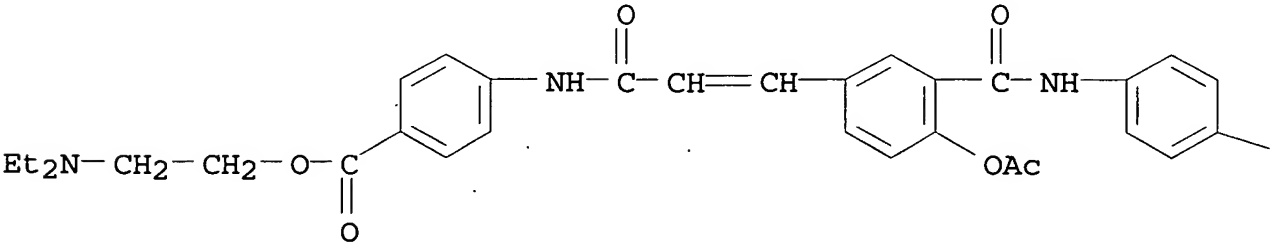
PAGE 1-B



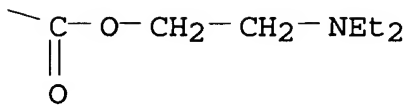
RN 150253-46-6 ZCA

CN Benzoic acid, 4-[[3-[4-(acetyloxy)-3-[[[4-[[2-(diethylamino)ethoxy]carbonyl]phenyl]amino]carbonyl]phenyl]-1-oxo-2-propenyl]amino]-, 2-(diethylamino)ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



IT **150231-93-9P 150253-46-6P**
(prepn. of, as allergy inhibitor)

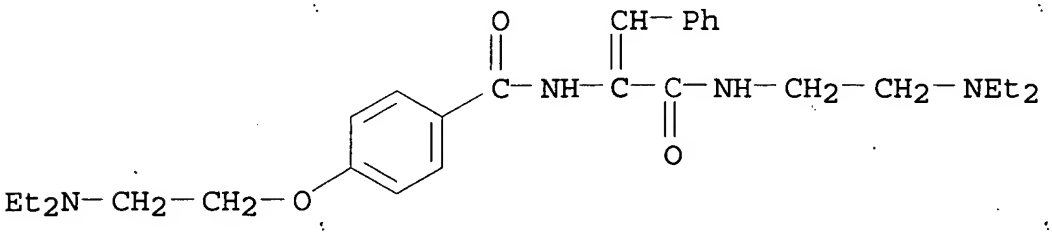
L25 ANSWER 19 OF 22 ZCA COPYRIGHT 2007 ACS on STN
69:67125 N-(2-Dialkylaminoethyl)-α-(acylamine)cinnamides. (E. Scheurich Pharmwerk G.m.b.H.). Brit. GB 1113569 19680515, 7 pp. (English). CODEN: BRXXAA. PRIORITY: DE 19651220 - 19661003 19661003.

GI For diagram(s), see printed CA Issue.

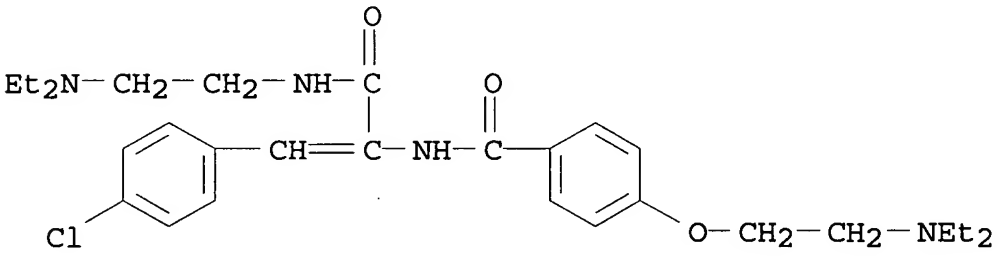
AB I are prepd. from azlactones II and H2NCH2CH2NR2. A soln. of 18.7 g. II (R1 = Me, R2 = R3 = H) in 300 ml. C6H6 is treated with 13 g. β-morpholinoethylamine at room temp. and the mixt. kept overnight to give 70% N-(β-morpholinoethyl)-α-acetylaminocinnamamide, m. 164-6° (Me2CO). Similarly prepd. are the following I (R or NR2, R1, R2, R3, m.p., and % yield given): morpholino, Me, H, MeO, 186-7°, 75; morpholino, Me, H, Cl, 180-1°, 71; morpholino, Me, H, AcO, 160-1°, 53; Me, Me, H, H, 139-41°, 60; Me, Me, H, H, 100-3°, 57; Et, Me, H, H, 138-9°, 70; Et, Me, H, Cl, 137-8°, 69; Et, Me, H, AcO, 136-7°, 72; Et, Me, MeO, MeO, 139-41°, 65; piperidino, Me, H, H, 171-2°, 58; piperidino, Me, H, Cl, 164-6°, 74; piperidino, Me, H, MeO, 146-8°, 80; Et, Ph, H, H, 146-7°, 83; Et, Ph, MeO, MeO, 117-19°, 51; morpholino, Ph, H, H, 170-1°, 82; Et, PhCH2, H, H, 114-16°, 75; Et, PhCH2, H, Cl, 131-2°, 76; Et, PhCH2, H, MeO, 104-6°, 65; morpholino, PhCH2, H, H, 154-5°, 58; Et, Ph2CH, H, H, 170-1°, 90; piperidino, Ph2CH, H, H, 156-8°, 81; and morpholino, Ph2CH, H, H, 153-5°, 80. Also prepd. were the following I [R = Et, R1 = p-(Et2NCH2CH2O)C6H4, R2 = H] (R3, m.p., and % yield given): H, 96-7°, 92; MeO, 116-18°, 75; and AcO, 99-102°, 62. Also prepd. were (m.p. and % yield given): N-(β-dimethylaminoisopropyl)-α-acetylaminocinnamamide, 130-1°, 64; and N-(β-morpholinoethyl)-α-acetylamino-o-methylcinnamamide, 162-3°, -.

IT **19380-72-4P 19380-73-5P 19380-74-6P**
19380-75-7P
(prepn. of)

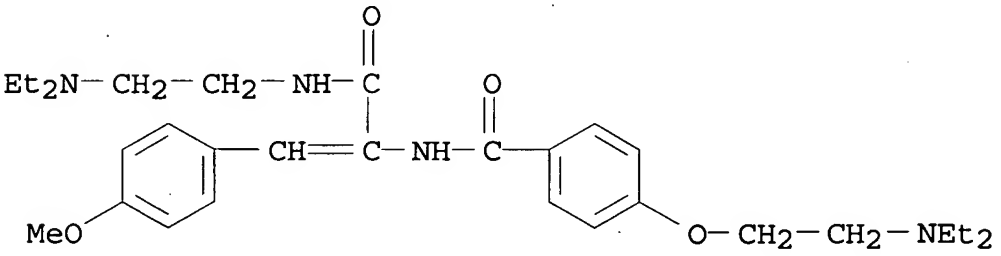
RN 19380-72-4 ZCA
CN Cinnamamide, α-[p-[2-(diethylamino)ethoxy]benzamido]-N-[2-(diethylamino)ethyl]- (8CI) (CA INDEX NAME)



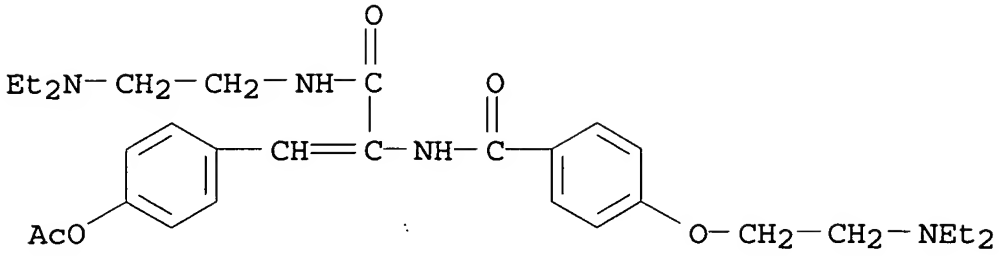
RN 19380-73-5 ZCA
CN Cinnamamide, p-chloro-α-[p-[2-(diethylamino)ethoxy]benzamido]-N-[2-(diethylamino)ethyl]- (8CI) (CA INDEX NAME)



RN 19380-74-6 ZCA
CN Cinnamamide, α-[p-[2-(diethylamino)ethoxy]benzamido]-N-[2-(diethylamino)ethyl]-p-methoxy- (8CI) (CA INDEX NAME)



RN 19380-75-7 ZCA
CN Cinnamamide, α-[p-[2-(diethylamino)ethoxy]benzamido]-N-[2-(diethylamino)ethyl]-p-hydroxy-, acetate (ester) (8CI) (CA INDEX NAME)



IT **19380-72-4P 19380-73-5P 19380-74-6P**
19380-75-7P
(prepn. of)

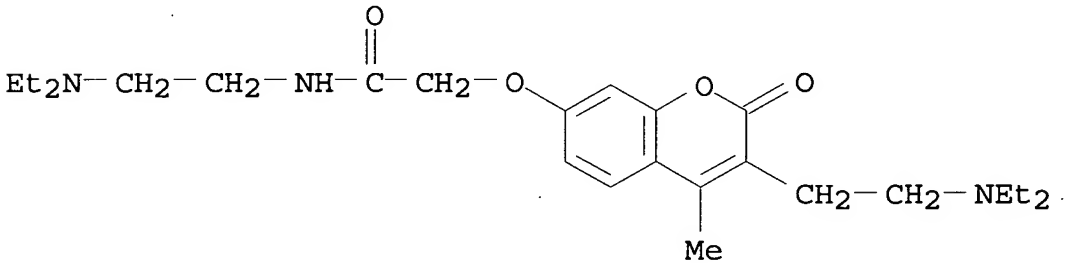
L25 ANSWER 20 OF 22 ZCA COPYRIGHT 2007 ACS on STN
65:56751 Original Reference No. 65:10568d-h,10569a 7-Hydroxycoumarin derivatives. Ritter, Heinrich; Beyerle, Rudi; Nitz, Rolf E. (Cassella Farbwerke Mainkur A.-G.). US 3259635 19660705, 6 pp. (Unavailable). APPLICATION: US 19640505. PRIORITY: US 19640505.
GI For diagram(s), see printed CA Issue.
AB The title compds. (I), which are coronary vasodilators, were obtained by treating 7-hydroxycoumarins with a halo compd. Thus, a soln. of 14.3 g. 4-phenyl-7-hydroxycoumarin (prepd. by condensing PhCOCH2CO2Et with resorcinol in concd. H2SO4) in 150 ml. MeCOEt was mixed with 10 g. anhyd. K2CO3, stirred 1 hr. at 70°, treated with 13 g. BrCH2CO2Et and 0.5 g. KI, and refluxed 8 hrs. with stirring to give 14 g. I (R = Ph, R1 = EtO, R2 = R3 = H), m. 137-8°. A soln. of 4 g. Ia (m. 154-6°) in 40 cc. H2O was sapond. by refluxing 4 hrs. to give Ia.HCl, m. 70-5°. A suspension of 14 g. 3-carbethoxymethyl-4-methyl-5,7-dihydroxycoumarin (prepd. by condensing phloroglucinol with di-Et acetylsuccinate) in 200 cc. MeCOEt was treated as above with 20 g. anhyd. K2CO3 and worked up to give 13 g. I(R1 = R2 = EtO2CH2C, R = Me, R3 = OCH2CO2Et), m. 110-12°. A mixt. of 10 g. Ia and 75 g. (CH2NH2)2 was stirred 15 hrs. at 20-5° to give 8 g. I (R = Me, R1 = H2NCH2CH2NHCOCH2; R2 = CH2CH2NEt2 R3 = H), m. 118-19°. A suspension of I (R = Me, R1 = OH, R2 = CH2CH2NEt2, R3 = H).HCl m 280 cc. MeCOEt and 20 g. K2CO3 was first treated as above and then with 9 g. ClCH2CONMe2 in 25 cc. MeCOEt and stirred 7 hrs. to give I (R = Me, R1 = Me2NCOCH2, R2 = Et2NCH2CH2, R3 = H), m. 203-6°. The following I (R3 = H) were similarly prepd. by the above procedures (R, R1, R2, and m.p. given): Me, CH2CO2Et, Bu, 78°; Me, CH2CO2Et, H, 98-100°; Me, CH2CO2Bu-tert; Ph, 113-15°; Me, CH2CO2Pr-iso, Ph, 138-40°; Ph, CH2CO2Bu-tert, Et, 122-3°; Ph, CH2CO2Pr-iso, Et, 124-5°; Me, CH2CO2Et, PhCH2, 117-20°; Me, CH2CO2Et, CH2CH:CH2, 42-4°; the following I.HCl (given as above): Me, Et, CH2CH2NEt2, 220-2°;

Me, CH2CH:CH2, CH2CH2NEt2, 198-201°; Me, Bu, C2H4NEt2, 288-90°; Me, CH2CH:CH2, β-(piperidino)ethyl, 220-2°; Ph, CH2CO2Et, CH2CH2NEt2, 158-60°; Me, CH2CO2Et, β-(piperidino)-ethyl, 208-9°; Me, CH2CO2Et, β-(morpholino)ethyl, 204-5°; Me, CH2CO2Et, β-(pyrrolidino)ethyl, 182-3°; Me, CH2CO2Et, Pr-NMe2, 180-2°; Me, CH2CO2Et, 1,3-bis(diethylamino)isopropyl, 176°; the following I amides (given as above): Me, CH2CONH2, CH2CH2NEt2, 186-7°; Me, CH2CONHCH2CH2NEt2, CH2CH2NEt2, 122-4°; Me, CH2CONHC6H12NH2, CH2CH2NEt2, 194°; Me, CH2CONH(CH2)3NMe2, CH2CH2NEt2, 120°; Me, CH2CONHBu, CH2CH2NEt2, 129°; Me, ZNHCOCH2 (Z = α-pyridyl), CH2CH2NEt2, 160-1°; Me, CH2CONBu2, CH2CH2NEt2, - (HCl salt, m. 129-30°).

IT **5614-98-2P**, Coumarin, 3-[2-(diethylamino)ethyl]-7-[[[2-(diethylamino)ethyl]carhamoyl]methoxy]-4-methyl-
(prepn. of)

RN 5614-98-2 ZCA

CN Coumarin, 3-[2-(diethylamino)ethyl]-7-[[[2-(diethylamino)ethyl]carbamoyl]methoxy]-4-methyl- (7CI, 8CI) (CA INDEX NAME)



IT **5614-98-2P**, Coumarin, 3-[2-(diethylamino)ethyl]-7-[[[2-(diethylamino)ethyl]carhamoyl]methoxy]-4-methyl-
(prepn. of)

L25 ANSWER 21 OF 22 ZCA COPYRIGHT 2007 ACS on STN

64:104093 Original Reference No. 64:19567f-h,19568a-b 7-Hydroxycoumarin derivatives. Ritter, Heinrich; Beyerle, Rudi; Nitz, Rolf E. (Cassella Farbwerke Mainkur, A.-G.). US 3243441 19630329, 5 pp. (Unavailable). APPLICATION: US 19640505. PRIORITY: US 19640505.

GI For diagram(s), see printed CA Issue.

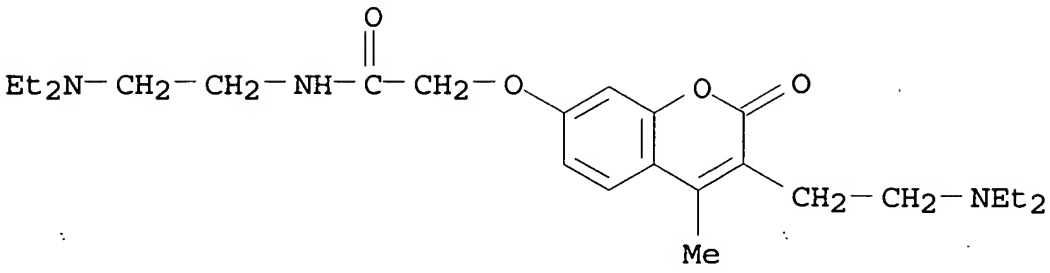
AB I, having specific vasocoronary dilating activity, without hypotensive side effects, of a prolonged nature were prepd. Thus, a mixt. of 14.3 g. 4-phenyl-7-hydroxycoumarin, 10 g. anhyd. K2CO3, and 150 ml. MeCOEt was heated 1 hr. at 70°. Following addn. of 13 g. BrCH2CO2Et and 0.5 g. KI, the mixt. was refluxed 8 hrs. with stirring to yield 71.8% Et 4-phenylcoumarin-7-oxyacetate, m.

137-8°. Analogously prepd. were (% yield and m.p. given): Et 3-butyl-4-methyl-coumarin-7-oxyacetate, 83.5, 78°; Et 4-methylcoumarin-7-oxyacetate, 72.5, 98-100°; tert-Bu 3-phenyl-4-methylcoumarin-7-oxyacetate, 69, 113-15% iso-Pr 3-phenyl-4-methylcoumarin-7-oxyacetate, 70, 138-40°; tert-Bu 3-ethyl-4-phenylcoumarin-7-oxyacetate, 64, 122-3°; iso-Pr 3-ethyl-4-phenylcoumarin-7-oxyacetate, 77, 124-5°; Et 3-benzyl-4-methylcoumarin-7-oxyacetate, 66, 117-20°; Et 3-allyl-4-methylcoumarin-7-oxyacetate, --, 42-4°, The following were prepd. as hydrochlorides (m.p. given): Et 3-(β-diethylaminoethyl)-4-methylcoumarin-7-oxyacetate, 154-6° (free base); Et 3-(β-diethylaminoethyl)-4-methylcoumarin-7-oxyacetate (II), 220-2°; allyl 3-(β-diethylaminoethyl)-4-methylcoumarin-7-oxyacetate, 198-201°; Bu 3-(β-diethylaminoethyl)-4-methylcoumarin-7-oxyacetate, 288-90°; allyl 3-(β-piperidinoethyl)-4-methylcoumarin-7-oxyacetate, 220-2°; Et 3-(β-diethylaminoethyl)-4-phenylcoumarin-7-oxyacetate, 158-60°; Et 3-(β-piperidinoethyl)4-methylcoumarinoxyacetate, 208-9°; Et 3-(β-morpholinoethyl)-4-methylcoumarinoxyacetate, 204-5°; Et 3-(β-pyrrolidinoethyl)-4-methylcoumarin-7-oxyacetate, 182-3°; Et 3-(β-dimethylaminopropyl)-4-methylcoumarin-7-oxyacetate, 180-2°; Et 3-[1,3-bis(diethylamino)-isopropyl]-4-methylcoumarin-7-oxyacetate, 176°. Sapon. of II gave quant. yield of the acid as HCl salt, m. 70-5°. Di-Et 3-carbethoxy-4-methylcoumarin-5,7-bis(oxyacetate) was synthesized in 57.5% yield, m. 110-12° (1:1 EtOAc-ligroine) Stirring 10 g. II with 75 g. $(H_2NCH_2)_2$ 15 hrs. at 20-25° afforded 8 g. 3-(β-diethylaminoethyl)-4-methylcoumarin-7-oxyacetic acid β-aminoethylamide, m. 118-19° (H_2O); concd. NH_3 yielded the corresponding amide, m. 186-7°. Similarly prepd. were the β-diethylaminoethylamide, m. 122-4°, the ω-aminohexylamide m. 194°, the γ-dimethylaminopropylamide, m. 120°, the butylamide, m. 129°, and α-pyridylamide, m. 160-1°. Using N,N-dimethylchloroacetamide there was obtained 59% 3-(β-diethylaminoethyl)-4-coumarin-7-oxyacetic acid diethylamide-HCl, m. 203-6°. The dibutylamide-HCl m. 129-30°.

IT **5614-98-2P**, Coumarin, 3-[2-(diethylamino)ethyl]-7-[[[2-(diethylamino)ethyl]carhamoyl]methoxy]-4-methyl-
(prepn. of)

RN 5614-98-2 ZCA

CN Coumarin, 3-[2-(diethylamino)ethyl]-7-[[[2-(diethylamino)ethyl]carbamoyl]methoxy]-4-methyl- (7CI, 8CI) (CA INDEX NAME)



IT **5614-98-2P**, Coumarin, 3-[2-(diethylamino)ethyl]-7-[[[2-(diethylamino)ethyl]carhamoyl]methoxy]-4-methyl-
(prepn. of)

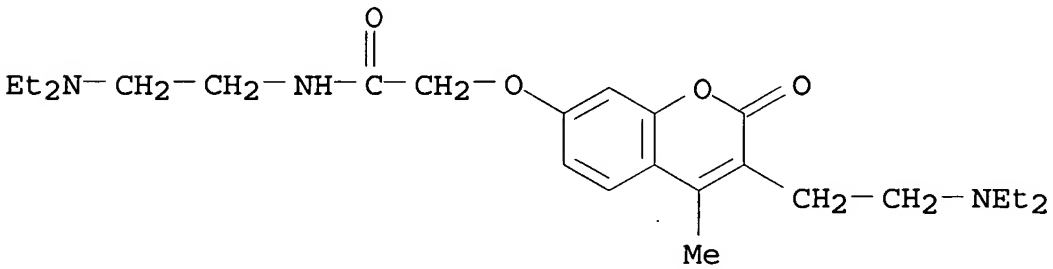
L25 ANSWER 22 OF 22 ZCA COPYRIGHT 2007 ACS on STN
59:62175 Original Reference No. 59:11438b-g Ethers of 7-hydroxycoumarins. (Cassella Farbwerke Mainkur, A.-G.). BE 621327 19630211, 26 pp. (Unavailable). PRIORITY: DE 19610812.
GI For diagram(s), see printed CA Issue.
AB I were synthesized by etherification of I (R3 = H). Thus, to 150 ml. MeCOEt were added 14.3 g. I (R1 = R3 = R4 = H, R2 = Ph) and 10 g. anhyd. K2CO3, the mixt. shaken 1 hr. at 70°, 13 g. BrCH2CO2Et and 0.5 g. KI were added, the whole was refluxed 8 hrs., filtered hot with suction, the filtrate concd. under reduced pressure, the residue extd. with CH2Cl2, the ext. washed with dil. NaOH and evapd., and the residue recrystd. from EtOAc to give 71.8% Et 4-phenyl-7-coumaryloxyacetate (I, R1 = R4 = H, R2 = Fh, R3 = CH2CO2Et), m. 137-8°. Similarly prepd. were I (R4 = H) (starting halide, R1, R2, R3, m.p., and % yield given): BrCH2CO2Et, Bu, Me, CH2CO2Et, 78°, 83.5; BrCH2CO2Et, H, Me, CH2CO2Et, 98-100°, 72.5; ClCH2CO2Bu-tert, Ph, Me, CH2CO2Bu-tert, 113-15°, 69; ClCH2CO2Pr-iso, Ph, Me, CH2CO2Pr-iso, 138-40°, 70; ClCH2CO2Bu-tert, Et, Ph, CH2CO2Bu-tert, 122-3°, 64; ClCH2CO2Pr-iso, Et, Ph, CH2CO2Pr-iso, 124-5°, 77; BrCH2CO2Et, PhCH2, Me, CH2CO2Et, 117-20°, 66; BrCH2CO2Et, CH2:CHCH2, Me, CH2CO2Et, 42-4°, -; BrCH2CO2Et, CH2CH2NEt2.HCl, Me, CH2CO2Et, 154-6°, 63; BrCH2CO2Et, CH2CH2NEt2.HCl, Me, Et, 220-2°, -. Also prepd. were I (R1, R2 R3, and m.p. given): CH2CH2NEt2.HCl, Me, CH2:CHCH2, 198-201°; CH2CH2NEt2.HCl, Me, Bu, 288-90°; β-piperidinoethyl-HCl, Me, CH2:CHCH2, 220-2°; CH2CH2NEt2.HCl, Ph, CH2CO2Et, 156-60°; β-piperidinoethyl, Me, CH2CO2Et, 208-9°; β-morpholinoethyl, Me, CH2CO2Et, 204-5°; β-pyrrolidinoethyl, Me, CH2CO2Et, 182-3°; γ-dimethylaminopropyl, Me, CH2CO2Et, 180-2°; 1,3-bis(diethylamino)isopropyl, Me, CH2CO2Et, 176°; I (R1 = CH2CH2NEt2.HCl, R2 = Me, R3 = CH2CO2H, R4 = H), m. 70-5°, was

prepd. quant. by sapon. of 4 g. Et ester in 40 ml. H2O at reflux 4 hrs. The etherification procedure described but without addn. of KI was used for the prepn. of the following I (R1, R2, R3, R4, and m.p. given): CH2CO2Et, Me, CH2CH2NH2, H, 126-9° (HCl salt), 66% yield; Bu, Me, CH2, CH2NEt2, H, 45-8°; Ph, Me, CH2CH2NEt2, H, 47-50°; H, Ph-CH2CH2NEt2, H, 75-6°; CH2CO2Et, Me, CH2CH2NEt2, OCH2CH2NEt2, 135-7° (HCl salt); CH2CO2Et, Me, CH2CO2Et, OCH2CO2Et, 110-12°; CH2CO2Et, Me, CH2CO2Et, H; 82-4° (75% yield); CH2CO2Et, Me, CH2CH:CH2, OCH2CH:CH2, 71-2° (67% yield); H, Me, CH2CH: CH2, H, 96-7° (83% yield). Treatment of 10 g. I (R1 = CH2CH2NEt2.HCl, R2 = Me, R3 = CH2CO2Et, R4 = H) with 75 g. H2NCH2CH2NH2 15 hrs. at 20-5° gave a colorless ppt. of I (R1 = CH2CH2NEt2, R2 = Me, R3 = CH2CONHCH2CH2NH2, R4 = H), m. 118-19°. Similarly prepd. were I (R1 = CH2CH2NEt2, R2 = Me, R4 = H) (R3 and m.p. given): CH2CONH2, 186-7°; CH2CONHCH2CH2NEt2, 122-4°; CH2CONH(CH2)6NH2, 194°; CH2CONH(CH2)3NMe2, 120°; CH2CONHBu, 129°; and CH2CONHZ (Z = α-pyridyl), 160-1°. I (R1 = CH2CH2NEt2.HCl, R2 = Me, R3 = CH2CONMe2, R4 = H), m. 203-6° was obtained in 59% yield by shaking 18.7 g. I (R1 = CH2CH2NEt2.HCl, R2 = Me, R3 = OH, R4 = H) and 20 g. anhyd. KI in 280 ml. MeCOEt 4 hrs. at 70°, adding dropwise 9 g. N,N-dimethylchloroacetamide in 25 ml. MeCOEt, and shaking the mixt. 8 hrs. at 70°. Also by this method was prepd. I (R1 = CH2CH2NEt2.HCl, R2 = Me, R3 = CH2CONBu2, R4 = H), m. 129-30°. The compds. prepd. are long-acting, coronary-specific vasodilators.

IT **5614-98-2P**, Coumarin, 3-[2-(diethylamino)ethyl]-7-[[[2-(diethylamino)ethyl]carhamoyl]methoxy]-4-methyl-
(prepn. of)

RN 5614-98-2 ZCA

CN Coumarin, 3-[2-(diethylamino)ethyl]-7-[[[2-(diethylamino)ethyl]carbamoyl]methoxy]-4-methyl- (7CI, 8CI) (CA INDEX NAME)



IT **5614-98-2P**, Coumarin, 3-[2-(diethylamino)ethyl]-7-[[[2-(diethylamino)ethyl]carhamoyl]methoxy]-4-methyl-
(prepn. of)